LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

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_X\Method\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029575.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	39	rBV2	172722	374444	21.99%	2.770%
2	1.368	43	46	52	rVV	188102	193737	11.38%	1.433%
3	1.752	103	109	120	rVB	678306	922905	54.20%	6.828%
4	1.953	137	142	150	rVB	73176	99104	5.82%	0.733%
5	2.215	180	185	194	rVB2	12540	21413	1.26%	0.158%
6	2.337	197	205	210	rBV	27208	54226	3.18%	0.401%
7	2.782	267	278	283	rBV	97448	218537	12.84%	1.617%
8	2.867	286	292	302	rVV	225772	462358	27.16%	3.421%
9	2.977	302	310	322	rVV2	41916	107567	6.32%	0.796%
10	3.105	322	331	343	rVB2	71268	174015	10.22%	1.287%
11	3.763	427	439	447	rBV5	10928	38827	2.28%	0.287%
12	4.306	515	528	540	rBV	179464	515748	30.29%	3.816%
13	4.428	540	548	557	rVB2	14674	40582	2.38%	0.300%
14	5.202	663	675	687	rVB4	9329	33696	1.98%	0.249%
15	5.391	694	706	713	rBV	148198	438544	25.76%	3.244%
16	5.477	713	720	725	rVV2	80794	237734	13.96%	1.759%
17	5.556	725	733	745	rVB2	283418	800883	47.04%	5.925%
18	5.958	790	799	812	rBV	159309	431299	25.33%	3.191%
19	6.245	837	846	857	rVV4	33021	94797	5.57%	0.701%
20	6.361	857	865	876	rVB10	5596	21698	1.27%	0.161%
21	6.763	922	931	943	rBV	425996	1028040	60.38%	7.606%
22	7.171	994	998	1009	rVB3	12972	28859	1.69%	0.214%
23	7.379	1021	1032	1040	rBV6	6751	19698	1.16%	0.146%
24	8.147	1147	1158	1164	rBV	66243	119125	7.00%	0.881%
25	8.427	1198	1204	1211	rBV	32296	58868	3.46%	0.436%
26	8.507	1211	1217	1226	rVB	64342	107527	6.32%	0.796%
27	8.653	1234	1241	1249	rBV	845326	1337949	78.58%	9.898%
28	8.842	1266	1272	1281	rBV	46255	75228	4.42%	0.557%
29	8.958	1288	1291	1297	rVB	20828	31818	1.87%	0.235%
30	9.049	1297	1306	1316	rVV	23509	41154	2.42%	0.304%
31	9.165	1319	1325	1333	rVB	19438	29341	1.72%	0.217%
32	9.458	1365	1373	1386	rBV2	43593	75653	4.44%	0.560%
33	9.567	1386	1391	1395	rBV2	20109	32635	1.92%	0.241%
34	10.055	1459	1471	1477	rBV	865801	1191539	69.98%	8.815%
35	10.146	1482	1486	1492	rVV2	28883	41111	2.41%	0.304%
36	10.244	1496	1502	1508	rVV3	19941	40909	2.40%	0.303%

LSC Area Percent Report

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

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_X\Method\82X061822W.M
Title : SW846 8260

37	10.305	1508	1512	1517	rVB	40600	53783	3.16%	0.398%
38	10.421	1525	1531	1539	rVB6	14188	28355	1.67%	0.210%
39	10.646	1563	1568	1573	rVB2	12499	17103	1.00%	0.127%
40	10.793	1587	1592	1597	rBV2	10565	18759	1.10%	0.139%
41	10.963	1614	1620	1625	rVB2	25017	40688	2.39%	0.301%
42	11.085	1634	1640	1649	rVB	646129	845348	49.65%	6.254%
43	11.177	1649	1655	1665	rVB2	15634	28952	1.70%	0.214%
44	11.274	1665	1671	1674	rBV2	14024	20672	1.21%	0.153%
45	11.616	1720	1727	1736	rBV	49602	69417	4.08%	0.514%
46	11.890	1763	1772	1778	rBV6	10167	22208	1.30%	0.164%
47	12.024	1788	1794	1801	rBV	845280	1044477	61.35%	7.727%
48	12.244	1824	1830	1839	rBV	1435479	1702620	100.00%	12.596%
49	12.701	1900	1905	1912	rVB	45686	58780	3.45%	0.435%
50	13.292	1998	2002	2007	rVB	19020	23968	1.41%	0.177%

Sum of corrected areas: 13516698

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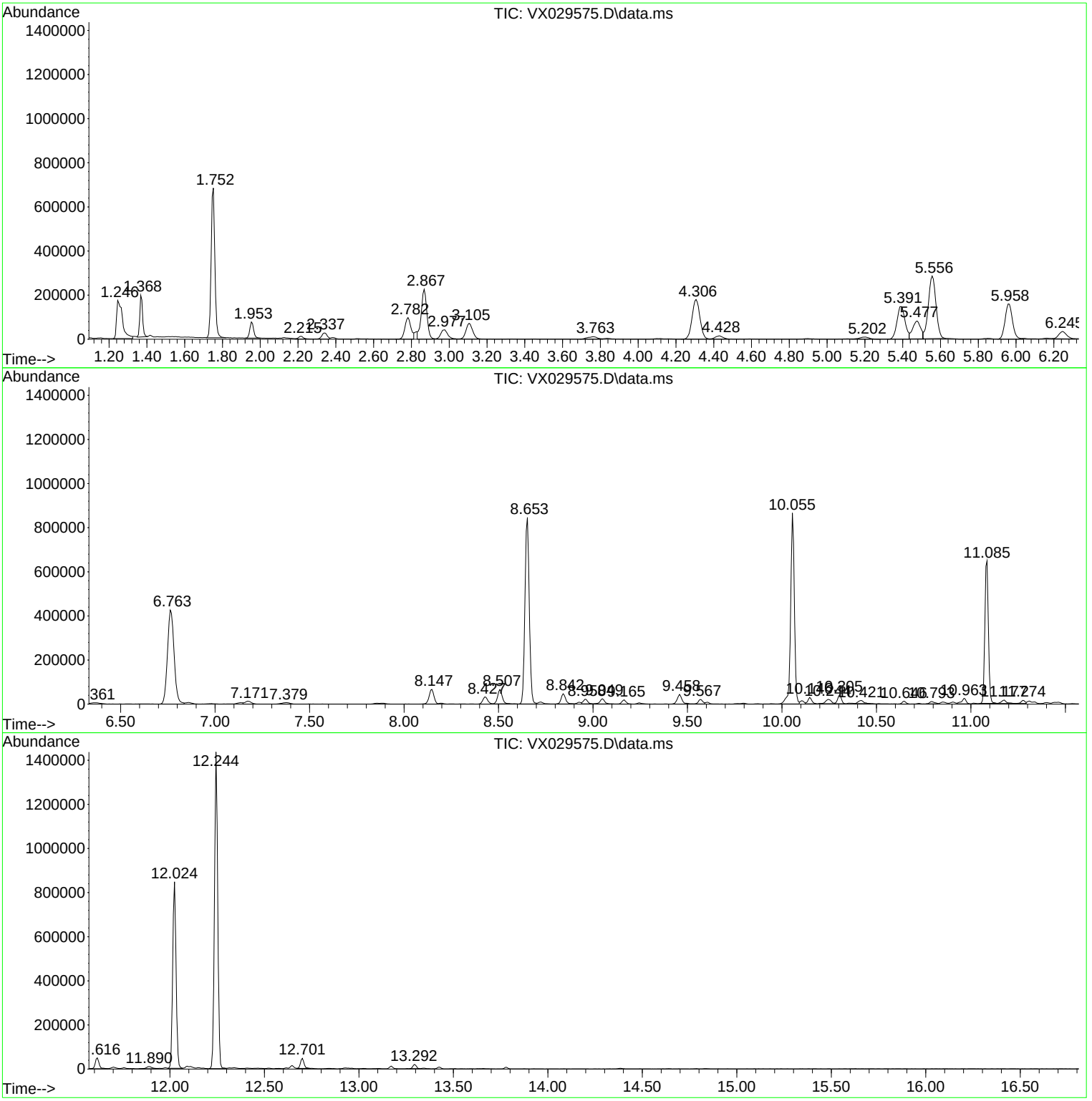
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

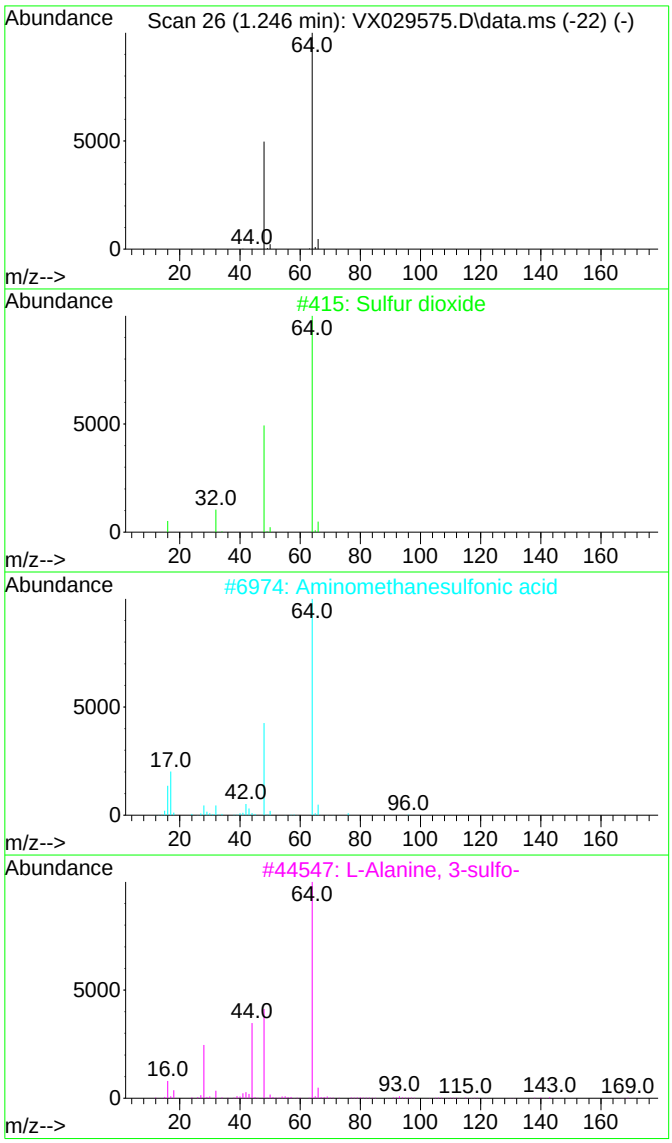
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

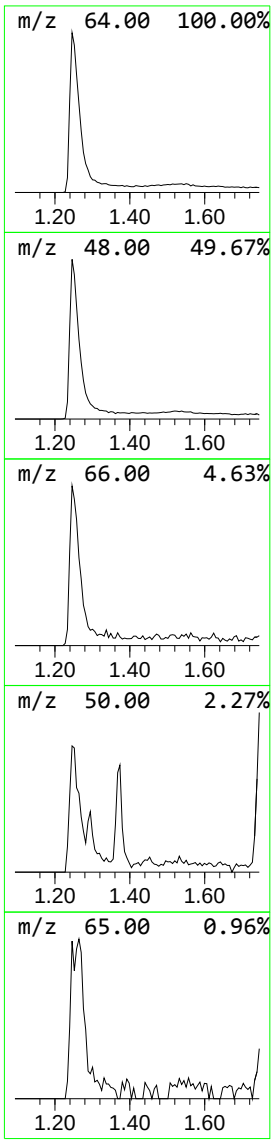
****

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	23.38 ug/l	374444	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

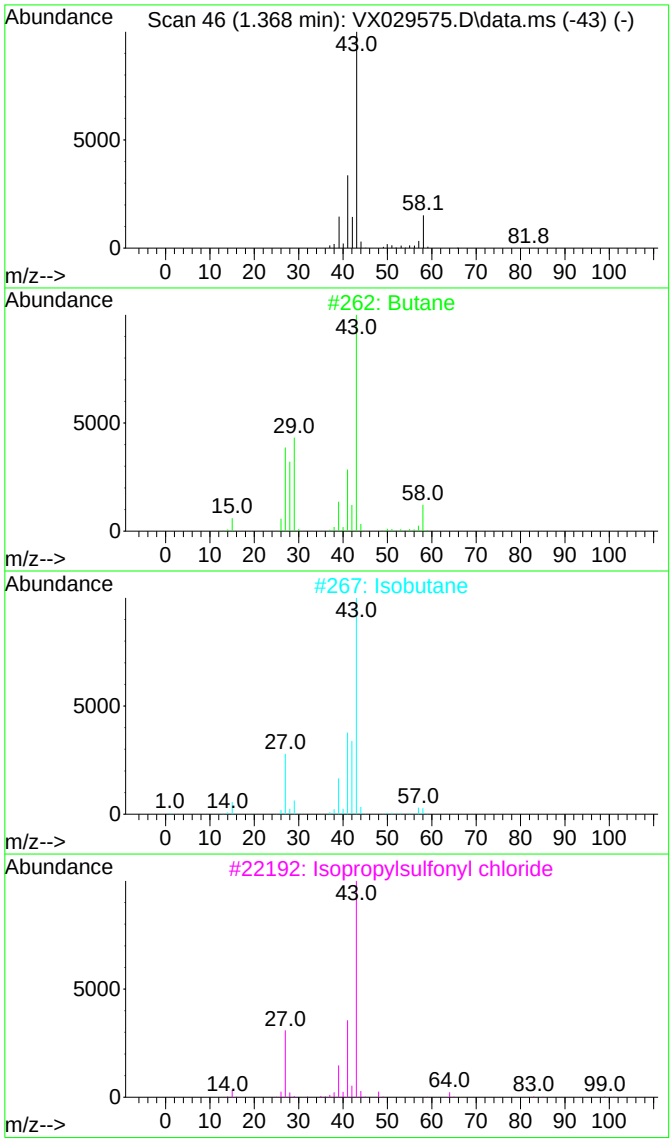
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

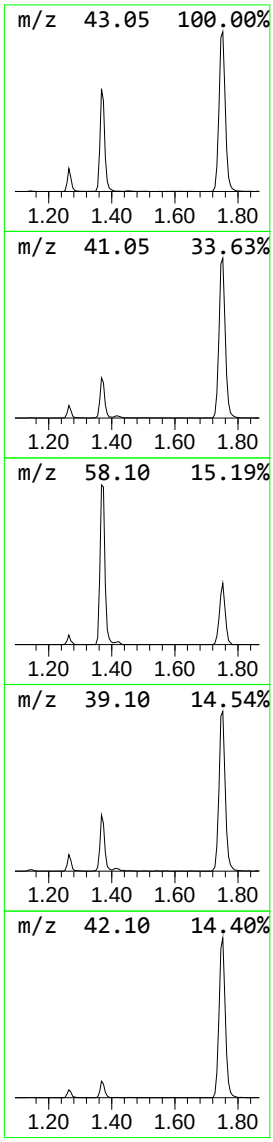
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	12.10 ug/l	193737	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isobutane	58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

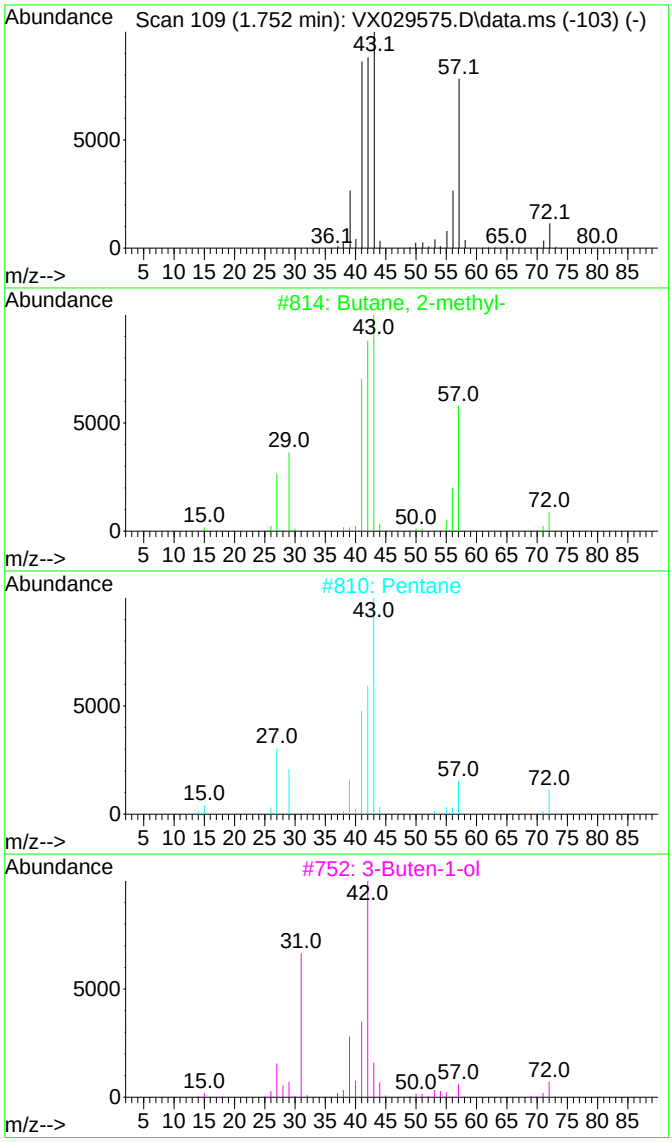
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

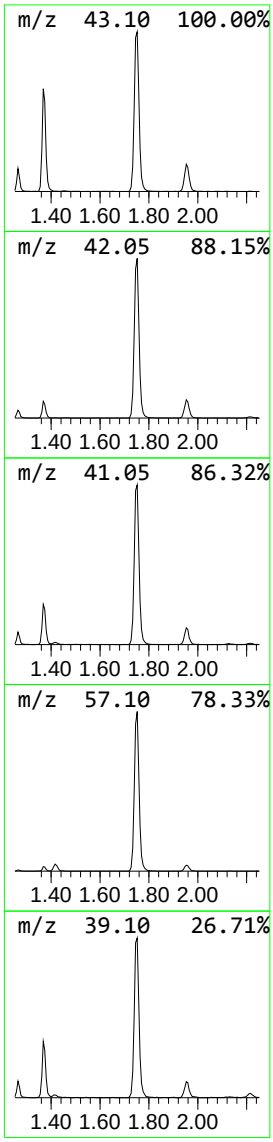
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	57.62 ug/l	922905	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	45
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	10
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

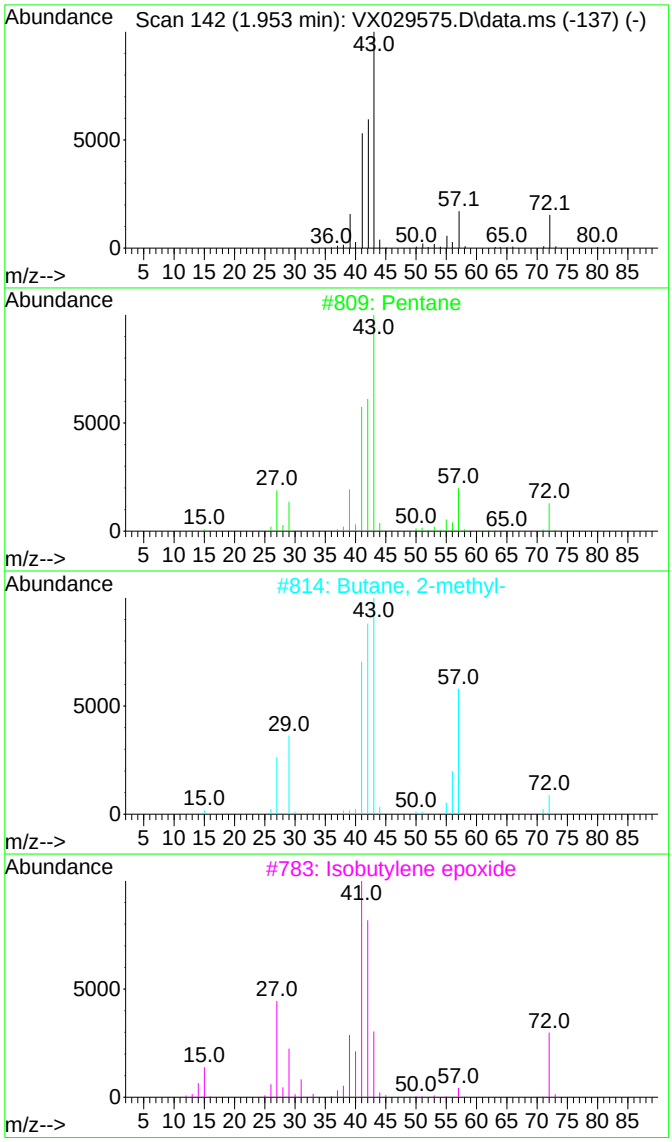
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

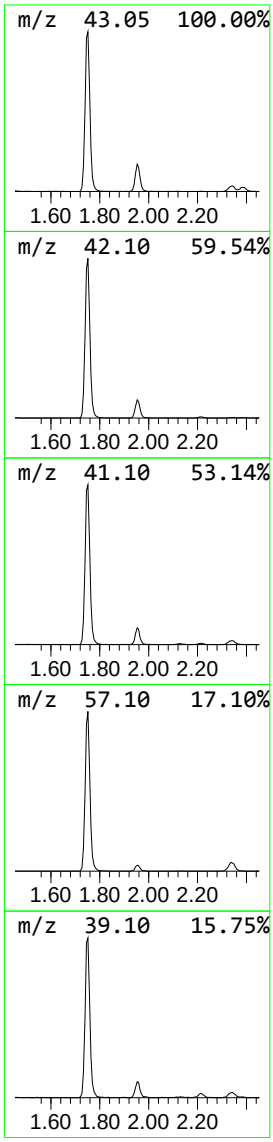
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.953	6.19 ug/l	99104	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	39
3	Isobutylene epoxide	72	C4H8O	000558-30-5	38
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	38
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

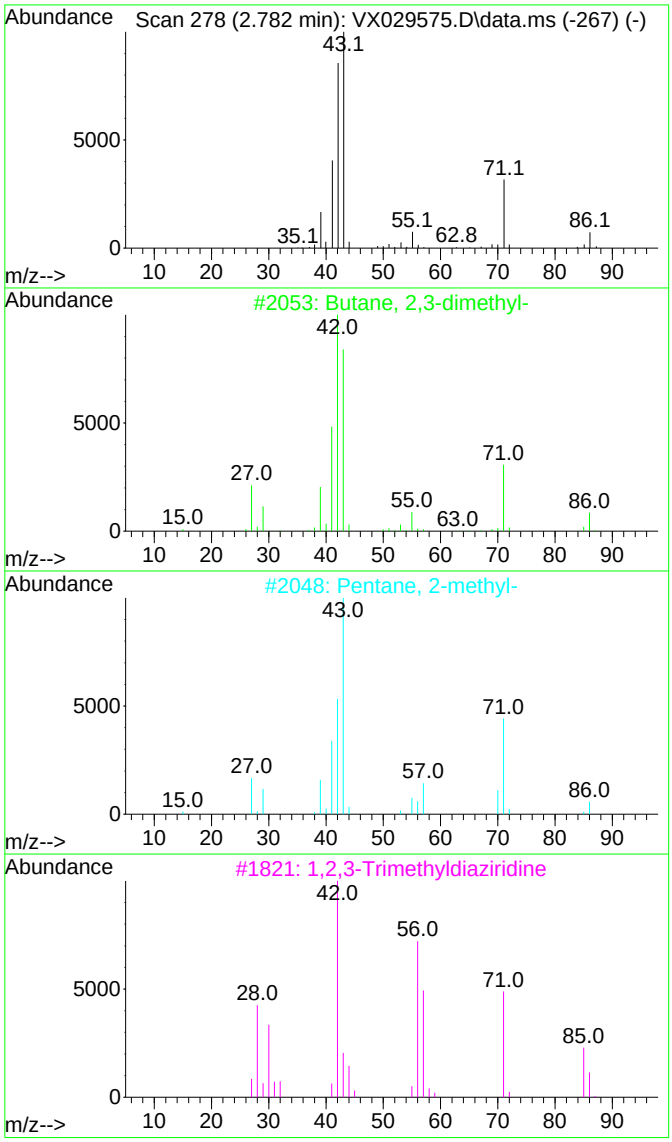
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

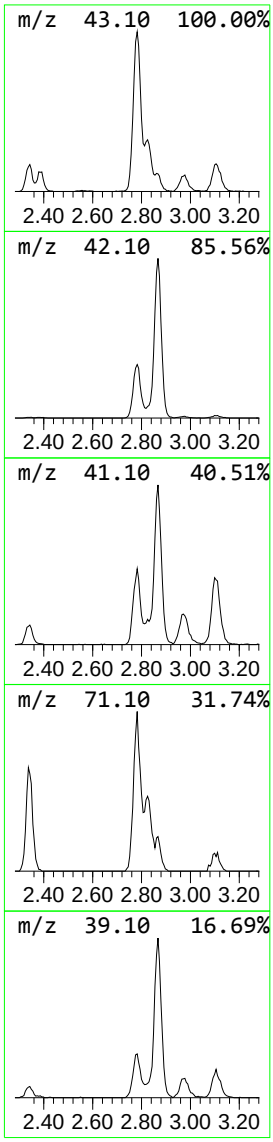
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	13.64 ug/l	218537	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	36
4	Pentane	72	C5H12	000109-66-0	23
5	Pyrrolidine	71	C4H9N	000123-75-1	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
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Operator : JC/MD
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

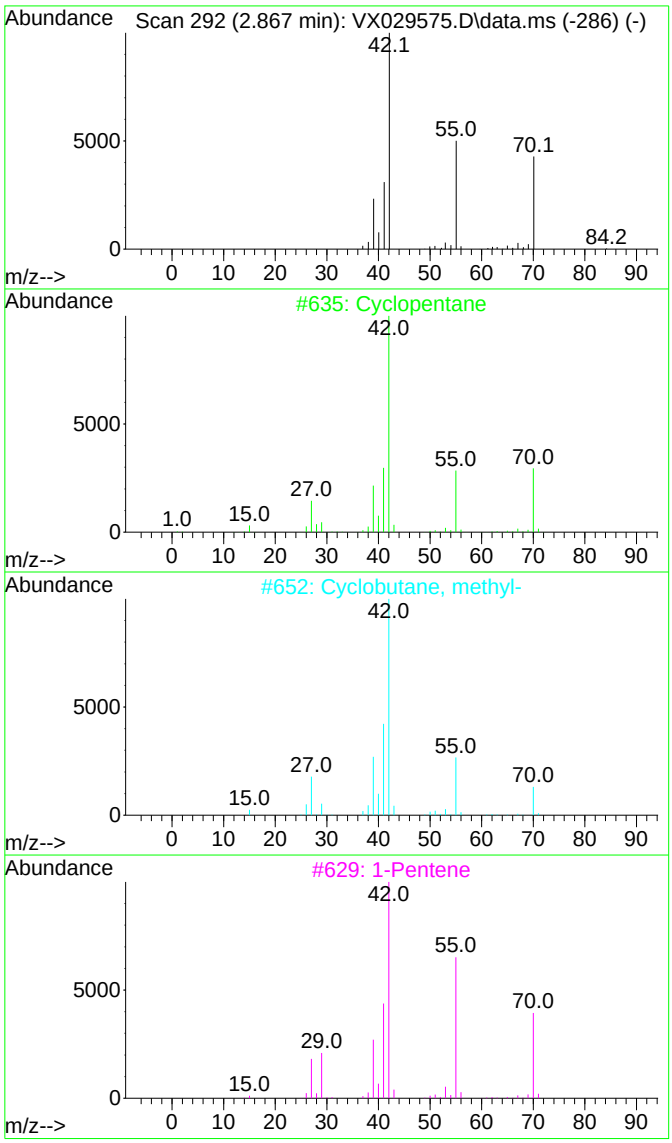
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

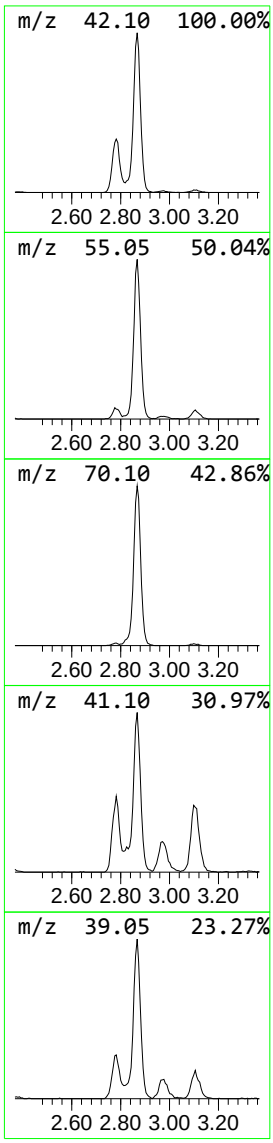
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	28.87 ug/l	462358	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	80
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3	1-Pentene	70	C5H10	000109-67-1	78
4	Methyl propargyl ether	70	C4H6O	000627-41-8	7
5	Ethoxyacetylene	70	C4H6O	000927-80-0	4





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

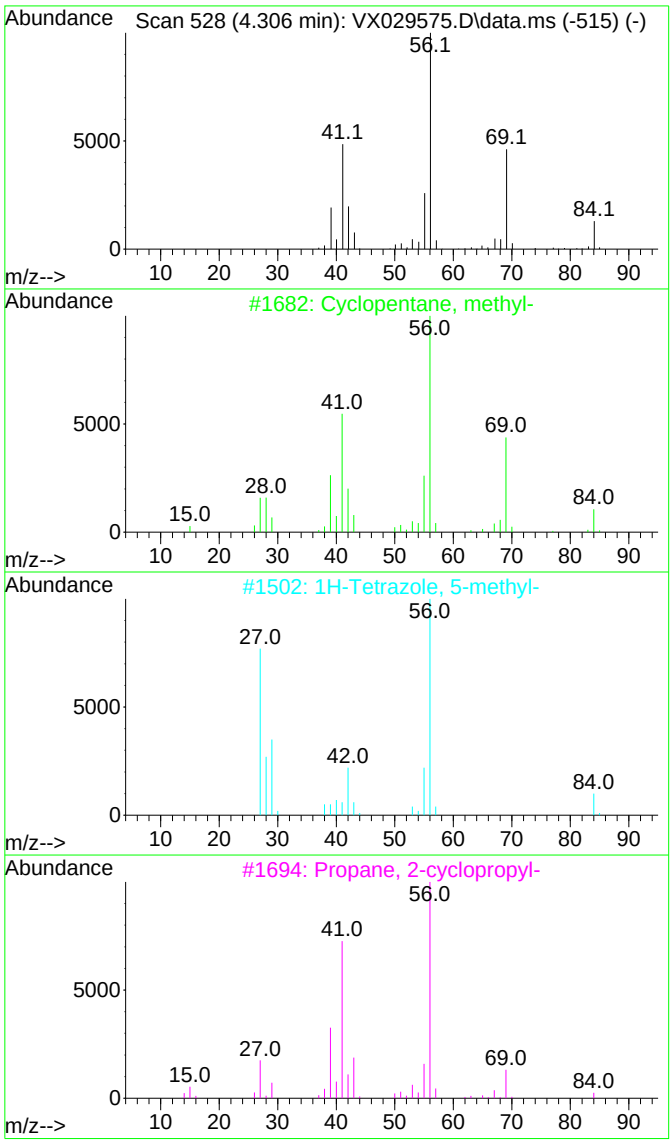
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

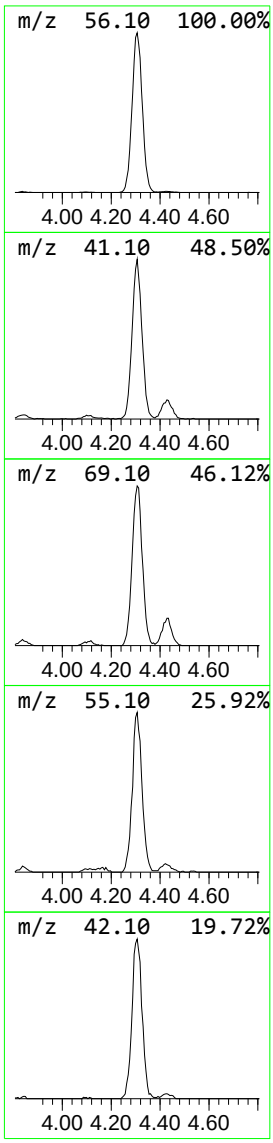
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	32.20 ug/l	515748	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	80
4	Cyclohexane	84	C6H12	000110-82-7	64
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

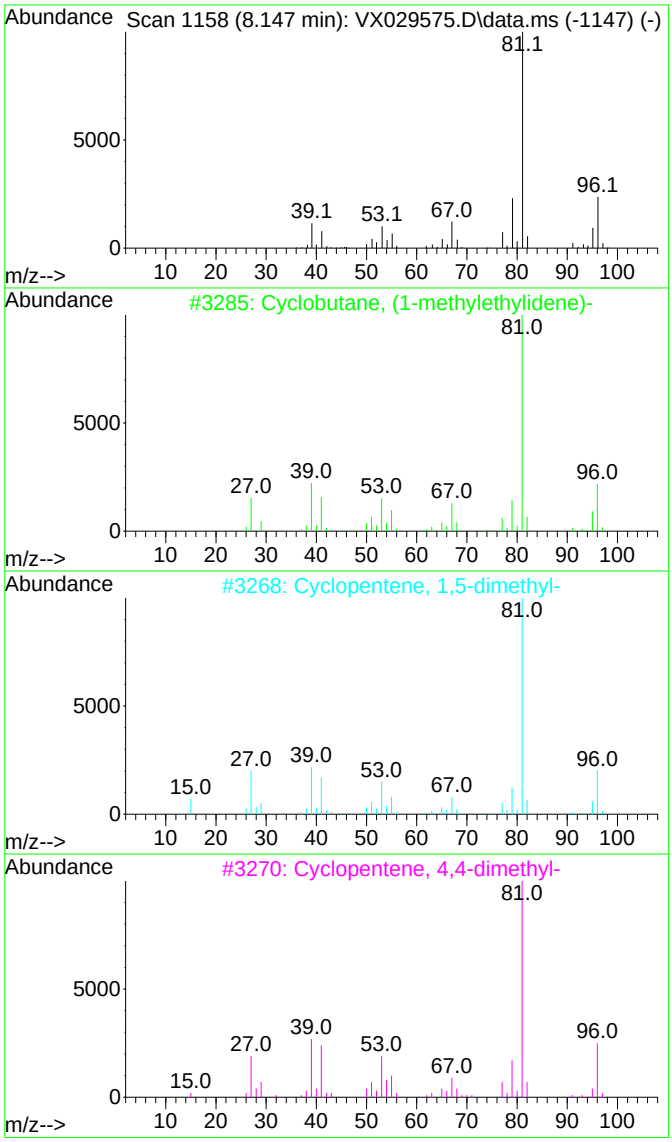
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

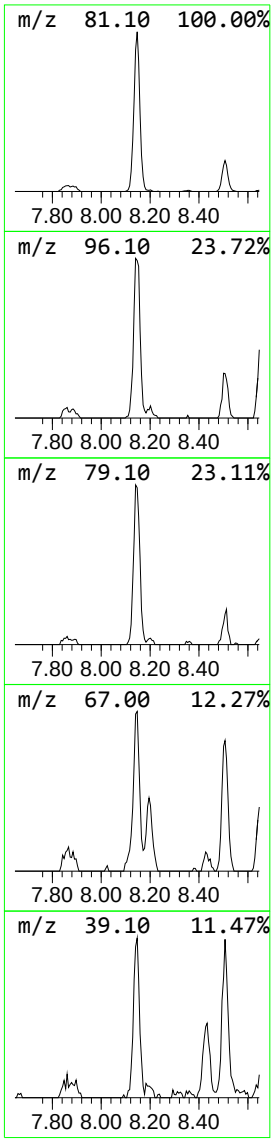
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclobutane, (1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.147	5.79 ug/l	119125	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
2	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	87
3	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	80
4	3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	78
5	Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

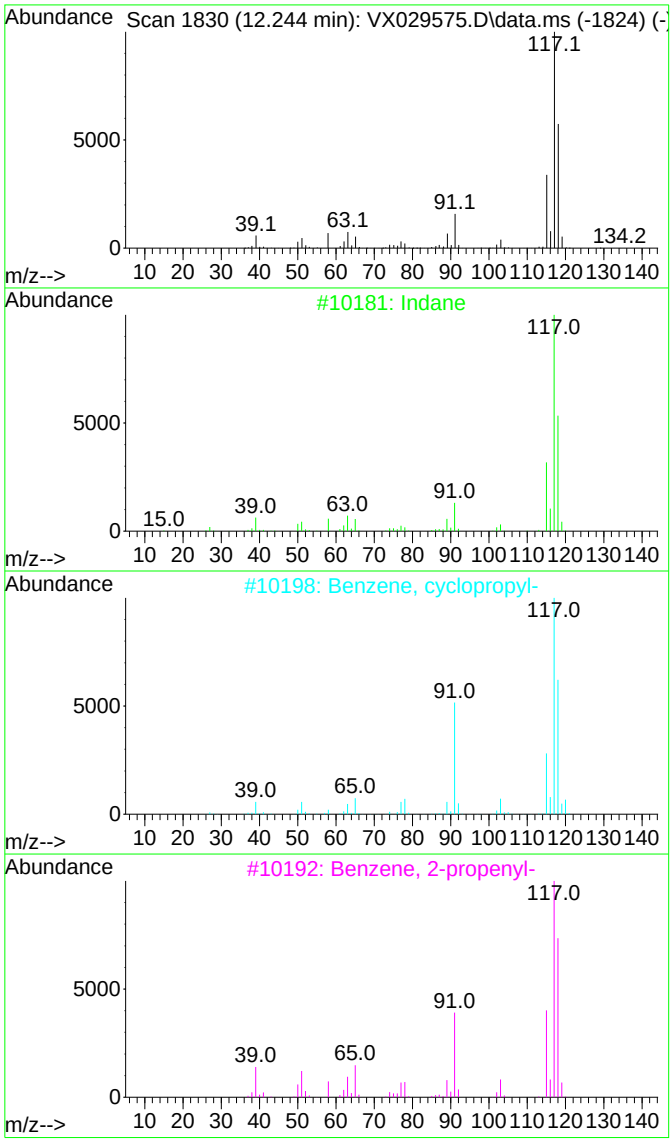
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

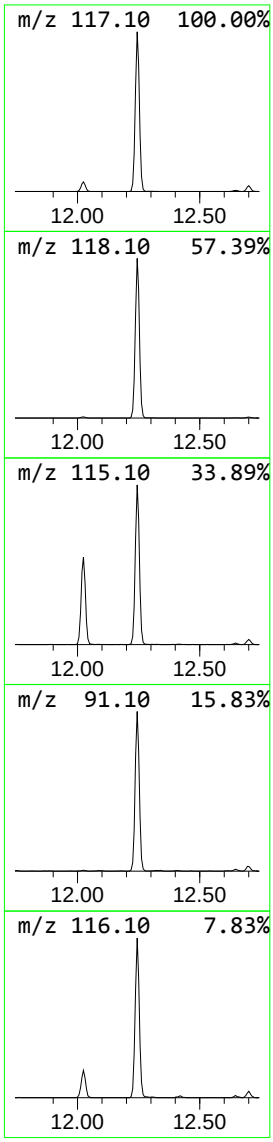
****

Peak Number 9 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	81.51 ug/l	1702620	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
5	Deltacyclene	118	C9H10	007785-10-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061822\
Data File : VX029575.D
Acq On : 18 Jun 2022 17:23
Operator : JC/MD
Sample : N3325-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-24

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.246	23.4	ug/l	374444	1	5.556	800883	50.0
Butane	1.368	12.1	ug/l	193737	1	5.556	800883	50.0
Butane, 2-methyl-	1.752	57.6	ug/l	922905	1	5.556	800883	50.0
Pentane	1.953	6.2	ug/l	99104	1	5.556	800883	50.0
Butane, 2,3-dim...	2.782	13.6	ug/l	218537	1	5.556	800883	50.0
Cyclopentane	2.867	28.9	ug/l	462358	1	5.556	800883	50.0
Cyclopentane, m...	4.306	32.2	ug/l	515748	1	5.556	800883	50.0
Cyclobutane, (1...	8.147	5.8	ug/l	119125	2	6.763	1028040	50.0
Indane	12.244	81.5	ug/l	1702620	4	12.024	1044480	50.0