LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

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\82X112222W.M
Title : SW846 8260

Signal : TIC: VX033140.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	43	rBV	64950	68573	6.25%	0.752%
2	1.374	43	47	52	rVV	289814	303436	27.64%	3.329%
3	1.752	103	109	120	rBV	838102	1097924	100.00%	12.045%
4	1.959	138	143	153	rVB2	81052	129983	11.84%	1.426%
5	2.215	180	185	194	rVB	50140	79967	7.28%	0.877%
6	2.343	194	206	212	rBV2	34313	66440	6.05%	0.729%
7	2.782	270	278	282	rBV	88179	188094	17.13%	2.063%
8	2.825	282	285	289	rVV	50188	105815	9.64%	1.161%
9	2.867	289	292	309	rVB2	76904	166988	15.21%	1.832%
10	3.105	321	331	345	rVB2	80006	177947	16.21%	1.952%
11	3.318	359	366	375	rVB4	7488	17297	1.58%	0.190%
12	3.733	426	434	443	rVB2	14870	35039	3.19%	0.384%
13	3.837	443	451	459	rBV4	18010	49270	4.49%	0.541%
14	4.105	483	495	504	rBV3	11684	30397	2.77%	0.333%
15	4.221	504	514	518	rVV4	6136	17388	1.58%	0.191%
16	4.306	518	528	541	rVV	142425	407592	37.12%	4.471%
17	4.422	541	547	564	rVB4	9030	28015	2.55%	0.307%
18	5.196	666	674	684	rVB	14760	44422	4.05%	0.487%
19	5.385	695	705	713	rBV	73549	215463	19.62%	2.364%
20	5.476	713	720	725	rVV	27071	69842	6.36%	0.766%
21	5.556	725	733	741	rVV	144533	386427	35.20%	4.239%
22	5.842	770	780	789	rBV7	5523	18135	1.65%	0.199%
23	5.958	789	799	807	rVV	75311	202814	18.47%	2.225%
24	6.043	807	813	823	rVV3	23099	64756	5.90%	0.710%
25	6.159	823	832	841	rVV5	11355	46276	4.21%	0.508%
26	6.257	841	848	857	rVV4	18481	57018	5.19%	0.626%
27	6.354	857	864	877	rVB4	8948	25415	2.31%	0.279%
28	6.763	921	931	942	rBV	236891	580058	52.83%	6.363%
29	6.848	942	945	954	rVB5	10370	26151	2.38%	0.287%
30	7.171	990	998	1008	rVB2	14675	33680	3.07%	0.369%
31	7.372	1021	1031	1042	rBV3	21650	64584	5.88%	0.709%
32	7.988	1122	1132	1143	rVB3	7423	18636	1.70%	0.204%
33	8.110	1143	1152	1154	rBV	15852	30620	2.79%	0.336%
34	8.141	1154	1157	1163	rVB	16982	29513	2.69%	0.324%
35	8.506	1210	1217	1225	rVB2	15716	26572	2.42%	0.292%
36	8.647	1225	1240	1248	rBV	343214	558495	50.87%	6.127%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

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\82X112222W.M
Title : SW846 8260

37	8.720	1248	1252	1258	rVB	7638	12809	1.17%	0.141%
38	10.055	1465	1471	1480	rBV	471426	631072	57.48%	6.923%
39	10.195	1489	1494	1504	rVV	141171	179658	16.36%	1.971%
40	10.305	1507	1512	1517	rVB	30139	40038	3.65%	0.439%
41	10.963	1615	1620	1625	rBV	21265	26953	2.45%	0.296%
42	11.079	1634	1639	1652	rBV	299700	386696	35.22%	4.242%
43	11.305	1669	1676	1684	rBV	36049	45429	4.14%	0.498%
44	11.402	1684	1692	1697	rBV	15913	20304	1.85%	0.223%
45	11.616	1721	1727	1734	rBV	176227	220980	20.13%	2.424%
46	11.756	1745	1750	1754	rBV	30581	36358	3.31%	0.399%
47	12.024	1788	1794	1799	rBV	480657	607450	55.33%	6.664%
48	12.085	1799	1804	1810	rVB	193500	246486	22.45%	2.704%
49	12.244	1824	1830	1837	rBV2	316109	390787	35.59%	4.287%
50	12.311	1837	1841	1849	rVV2	22475	33904	3.09%	0.372%
51	12.408	1852	1857	1862	rBV2	18956	24505	2.23%	0.269%
52	12.463	1862	1866	1873	rVB	39442	49422	4.50%	0.542%
53	12.530	1873	1877	1886	rVB	7031	11977	1.09%	0.131%
54	12.615	1886	1891	1894	rBV	84425	102160	9.30%	1.121%
55	12.701	1900	1905	1913	rVV2	79126	112546	10.25%	1.235%
56	12.847	1924	1929	1934	rBV	26584	33452	3.05%	0.367%
57	12.920	1934	1941	1945	rVV	62357	74068	6.75%	0.813%
58	12.963	1945	1948	1954	rVB2	9811	11928	1.09%	0.131%
59	13.170	1978	1982	1987	rVB	38465	45490	4.14%	0.499%
60	13.292	1997	2002	2007	rVB2	123699	161550	14.71%	1.772%
61	13.426	2019	2024	2031	rVB	15110	20672	1.88%	0.227%
62	13.579	2046	2049	2055	rVB3	8481	13392	1.22%	0.147%
63	13.664	2061	2063	2069	rVB3	7937	12158	1.11%	0.133%
64	13.780	2076	2082	2087	rBV	33235	45838	4.17%	0.503%
65	14.639	2219	2223	2229	rVB	19172	22954	2.09%	0.252%
66	14.780	2238	2246	2255	rBV	18813	25415	2.31%	0.279%

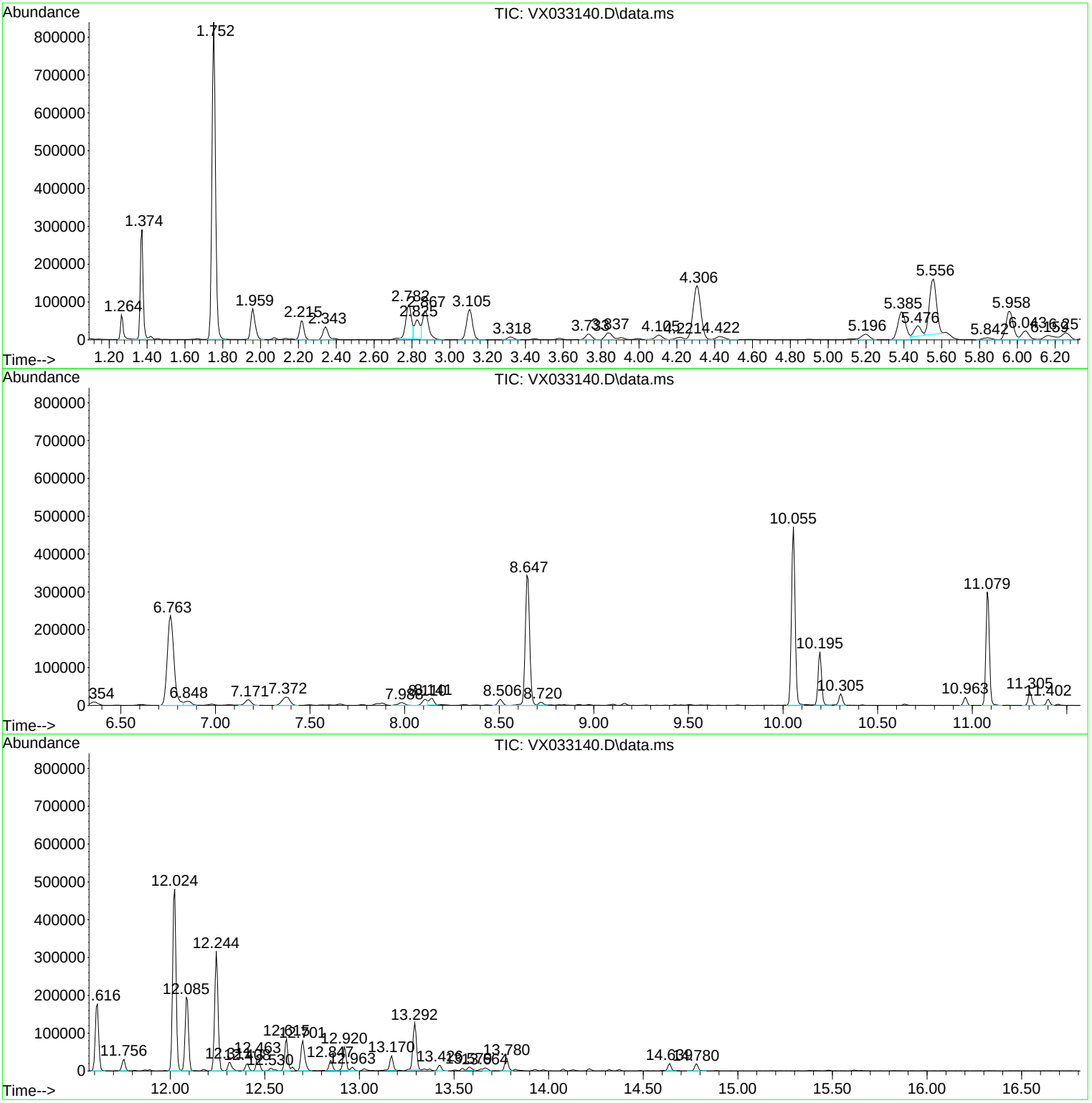
Sum of corrected areas: 9115493

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

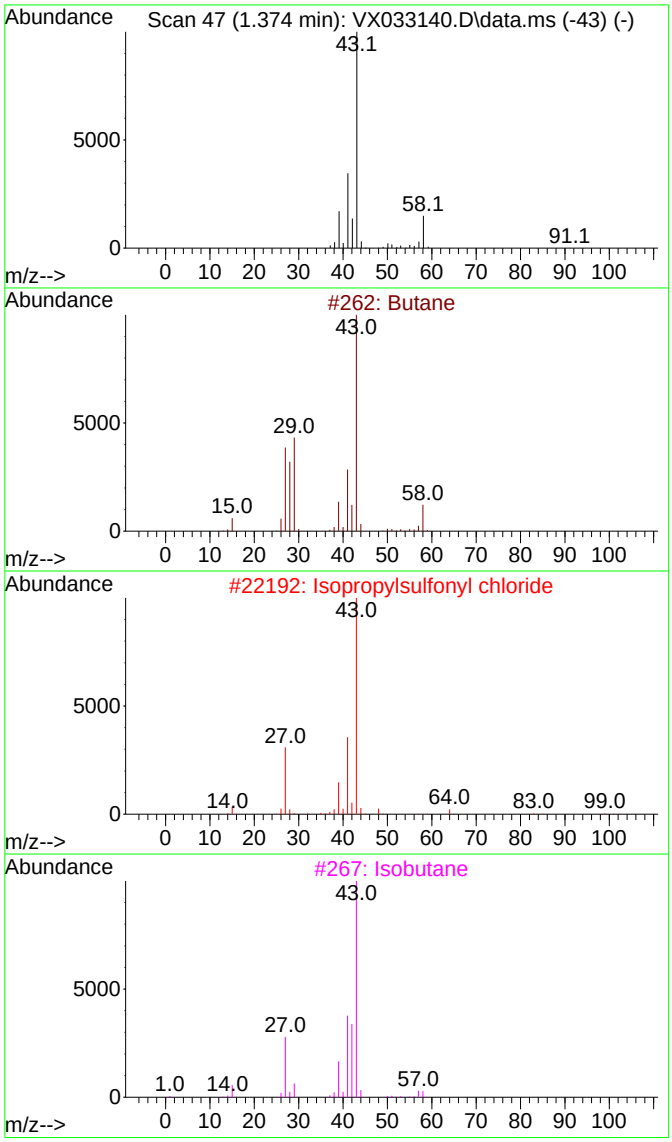
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

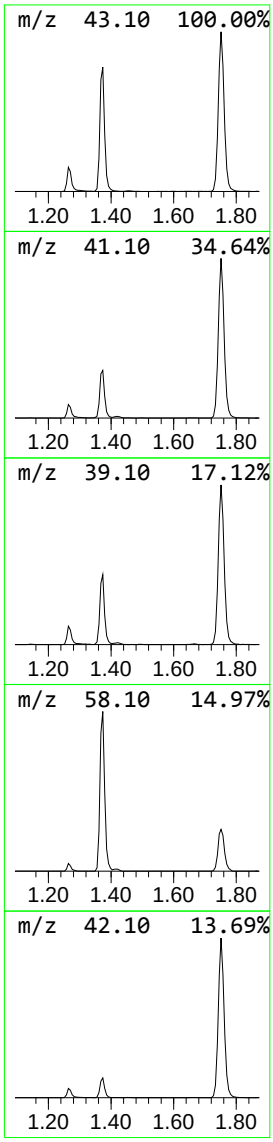
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	39.26 ug/l	303436	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Isobutane	58	C4H10	000075-28-5	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\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

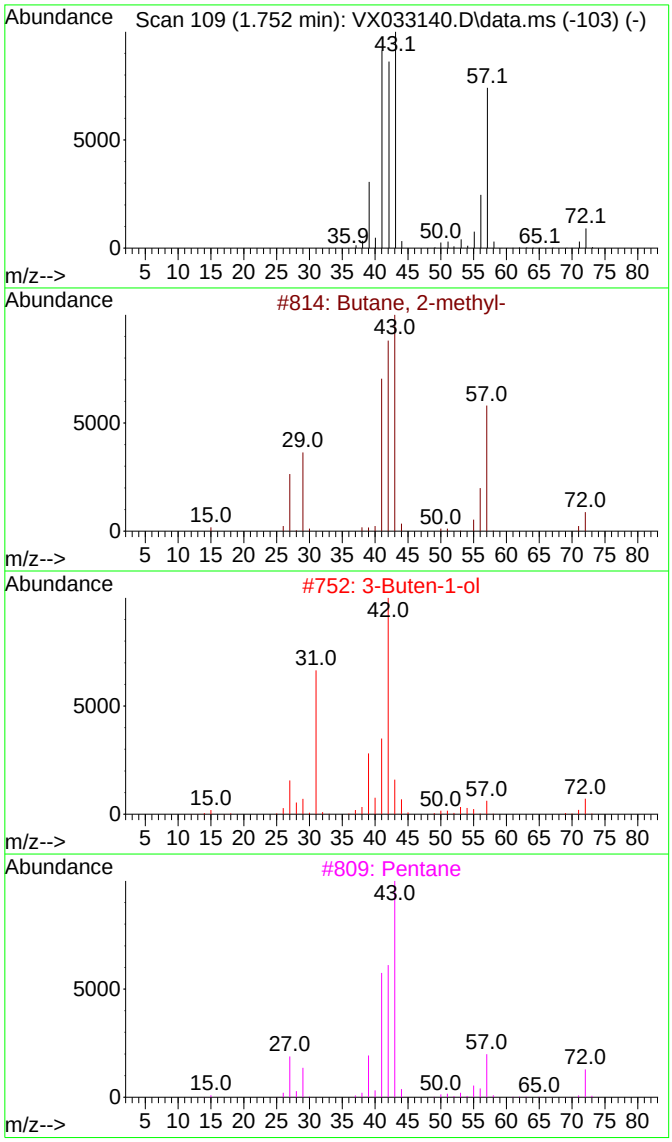
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

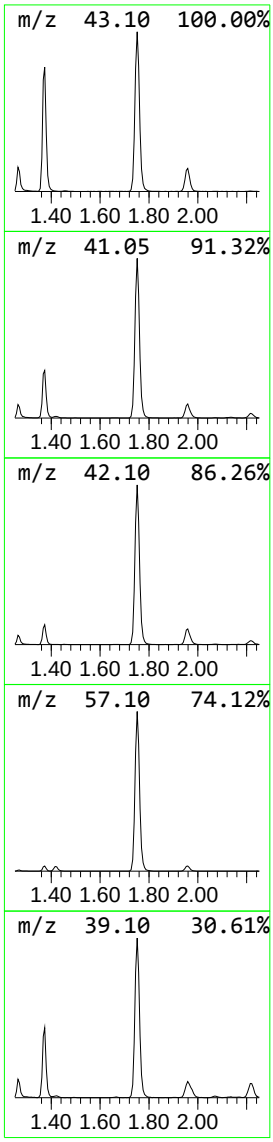
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	142.06 ug/l	1097920	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	33
4	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

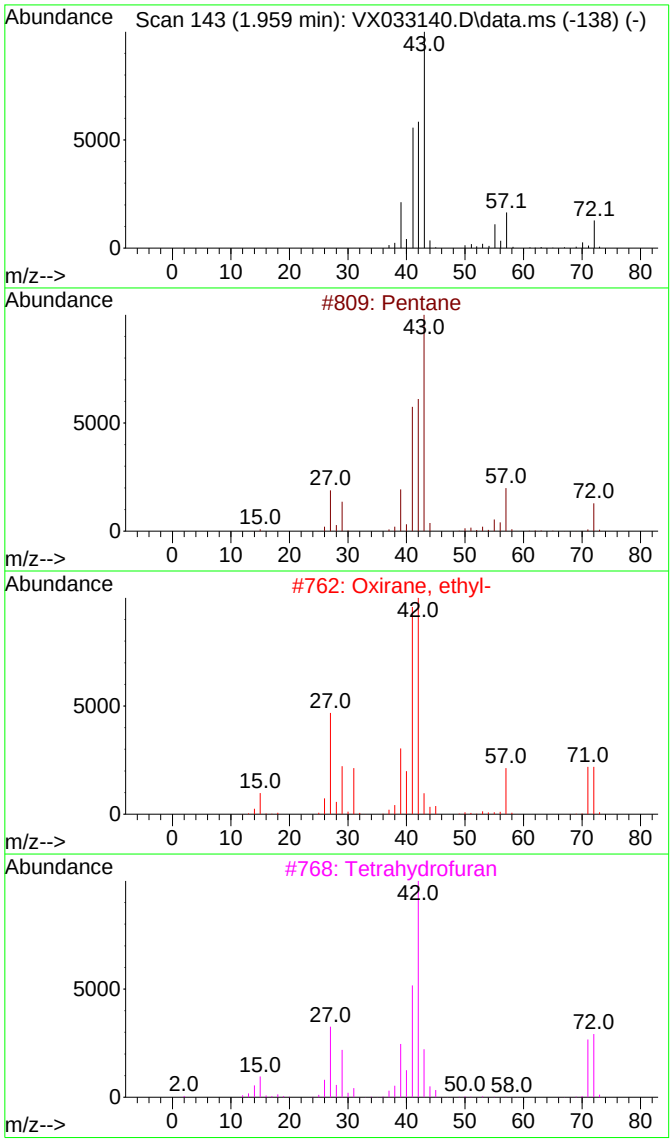
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

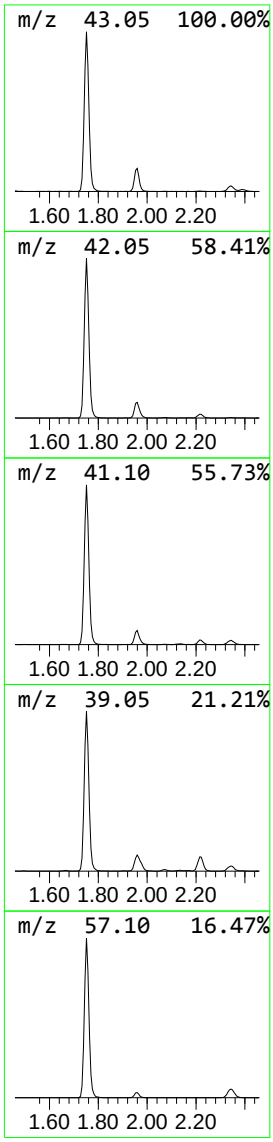
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	16.82 ug/l	129983	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	40
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

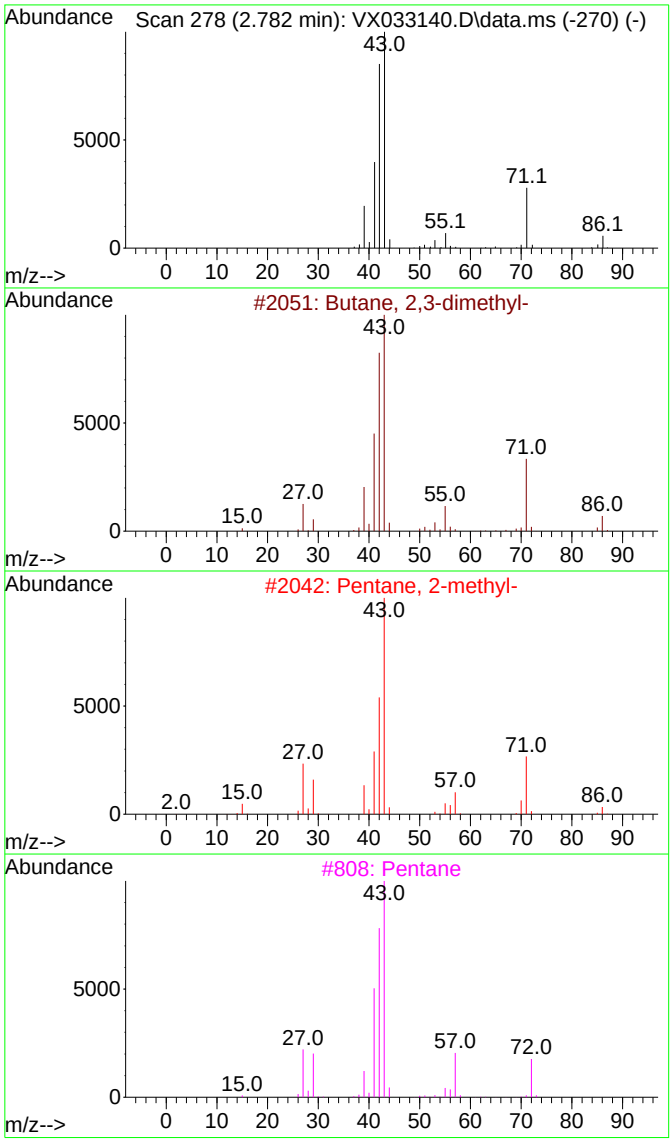
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

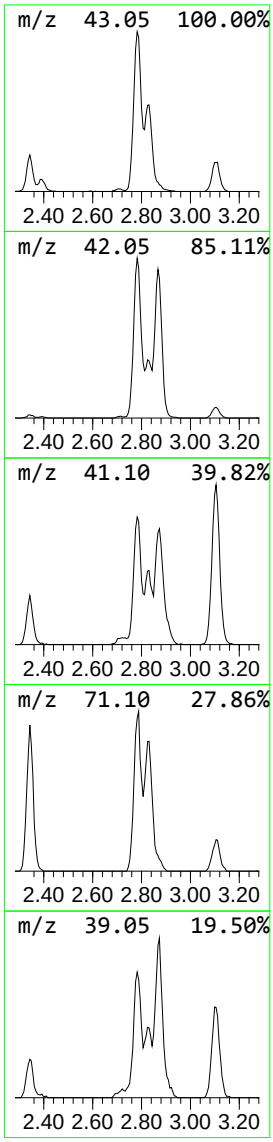
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	24.34 ug/l	188094	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	53
3	Pentane	72	C5H12	000109-66-0	45
4	Tetrahydrofuran	72	C4H8O	000109-99-9	38
5	Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

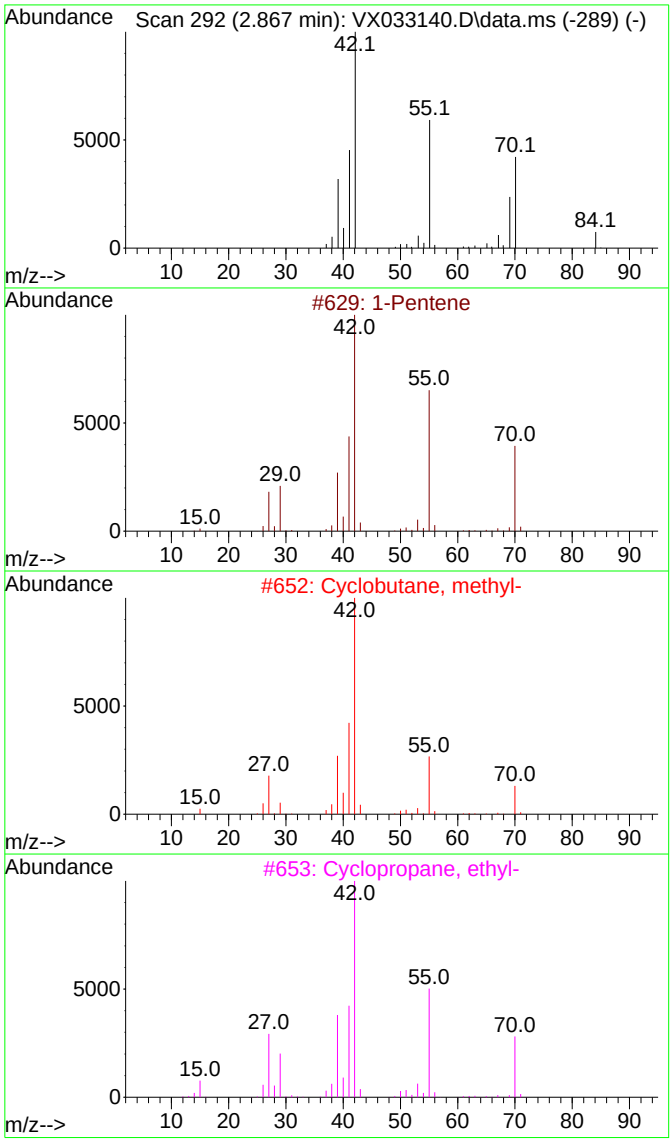
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

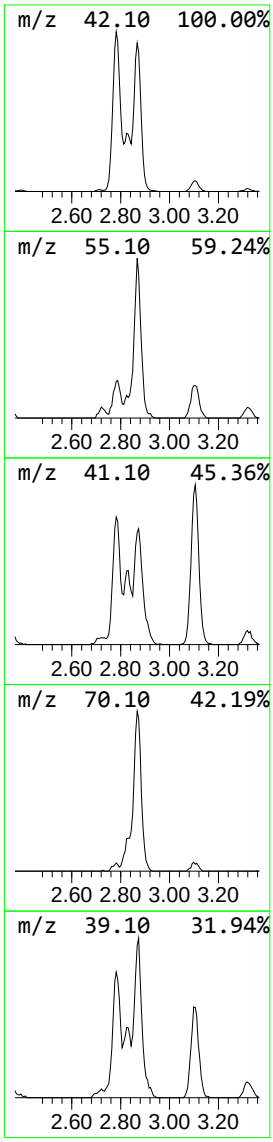
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Pentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	21.61 ug/l	166988	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	59
4	2-Pentene, (E)-	70	C5H10	000646-04-8	38
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

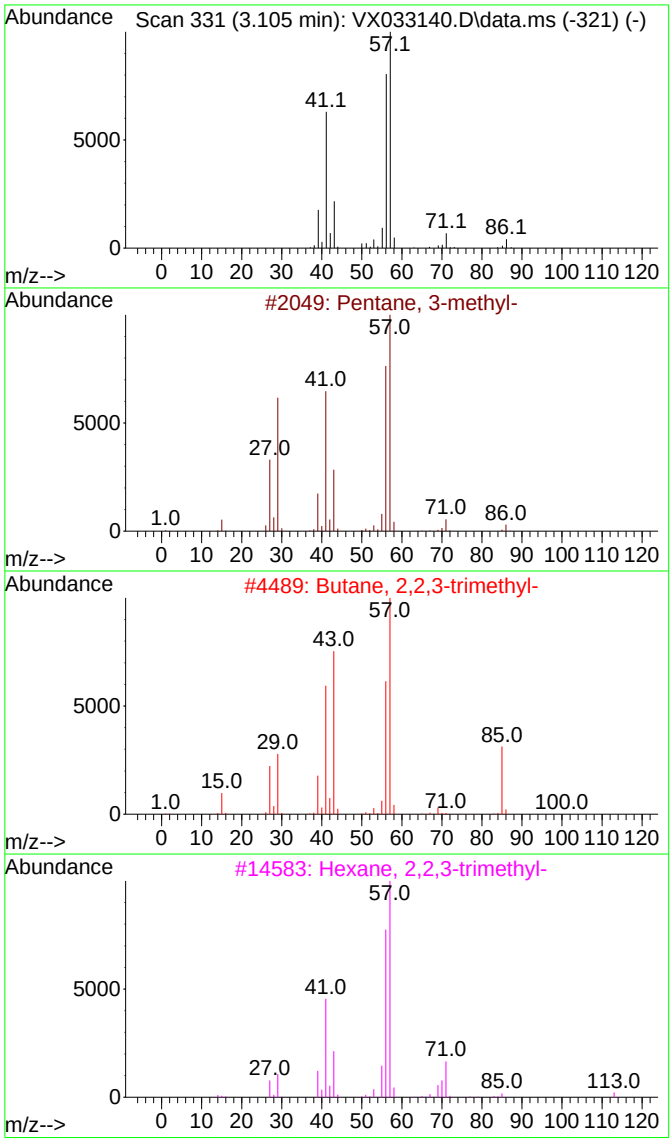
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

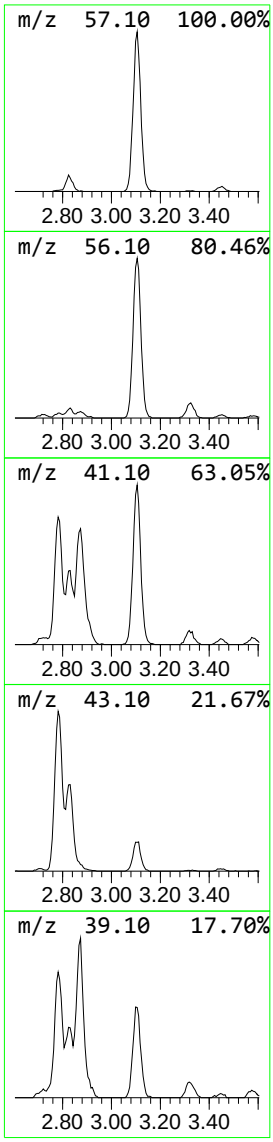
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	23.02 ug/l	177947	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

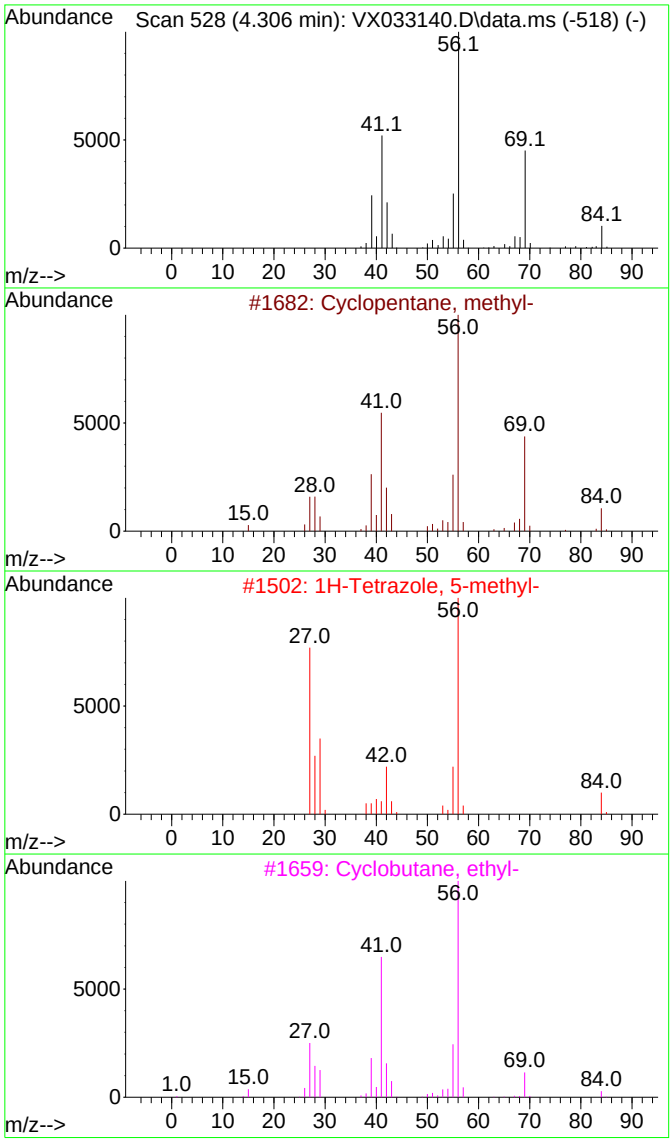
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

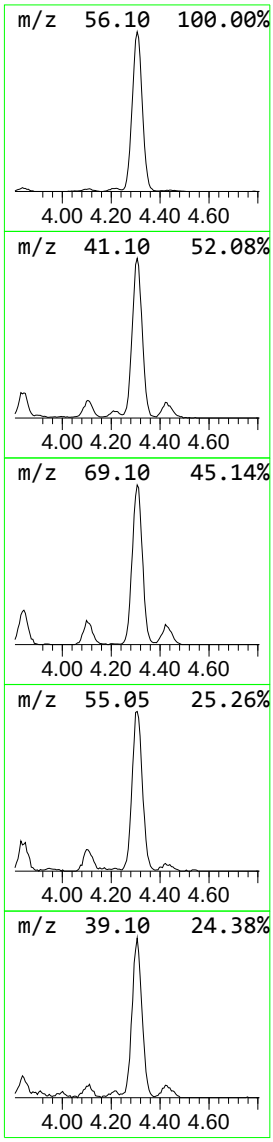
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	52.74 ug/l	407592	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	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	Cyclohexane	84	C6H12	000110-82-7	64
5	Cyclobutane	56	C4H8	000287-23-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

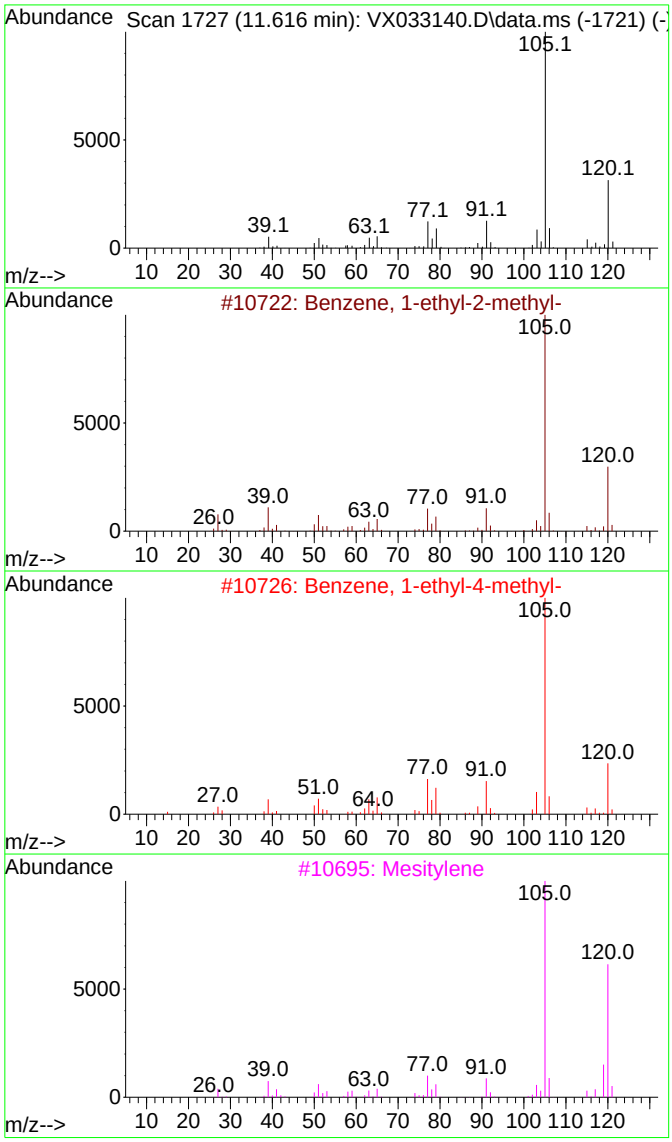
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

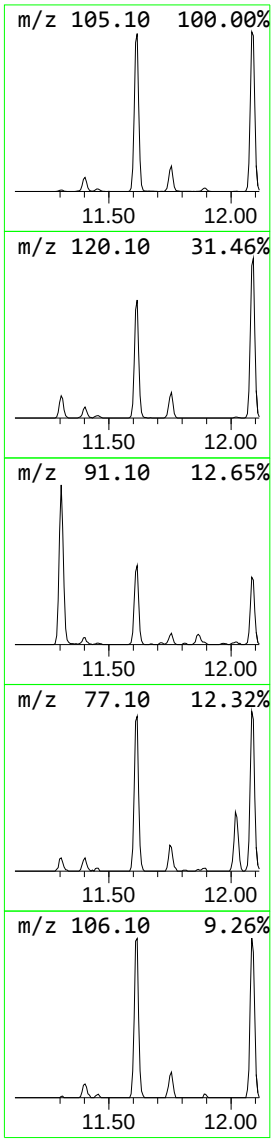
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	18.19 ug/l	220980	1,4-Dichlorobenzene-d4	12.024

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

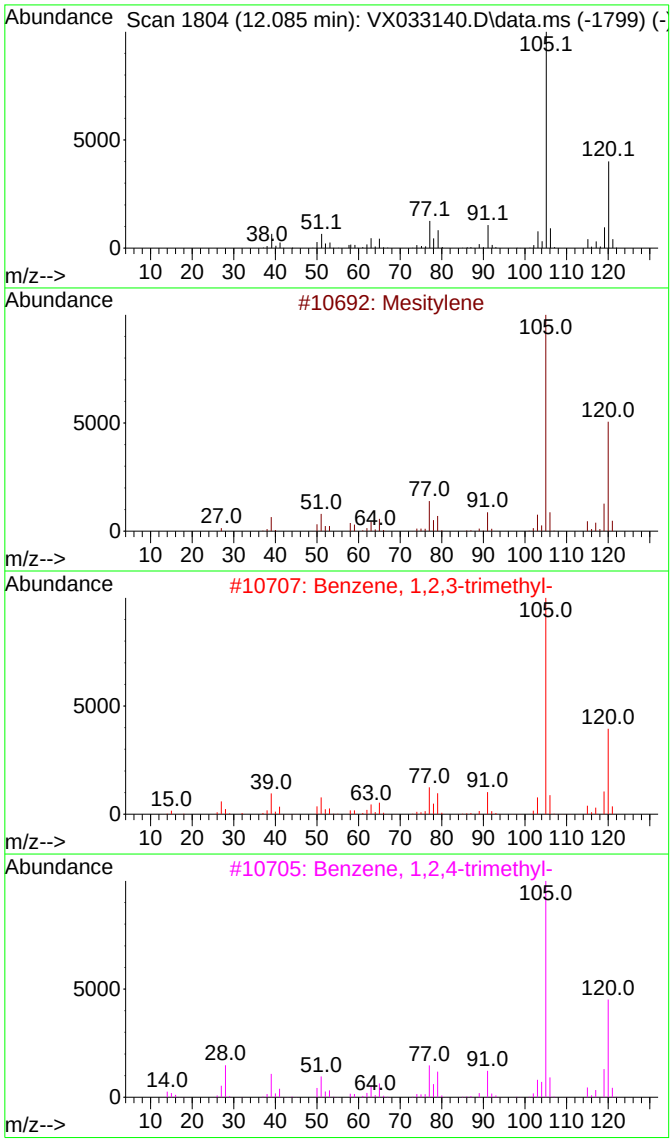
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

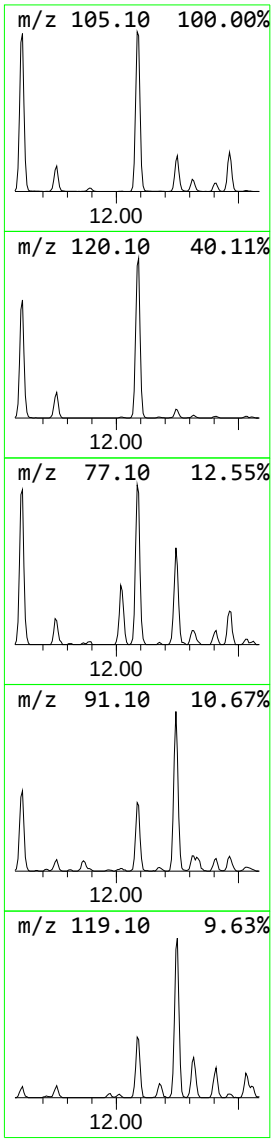
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	20.29 ug/l	246486	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

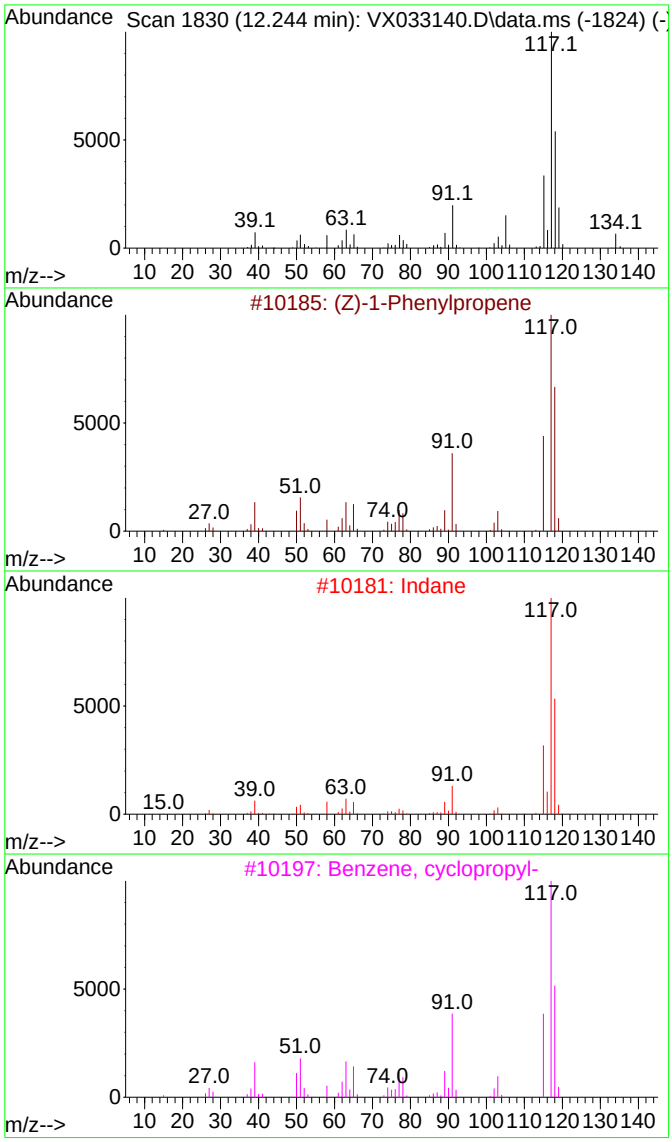
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

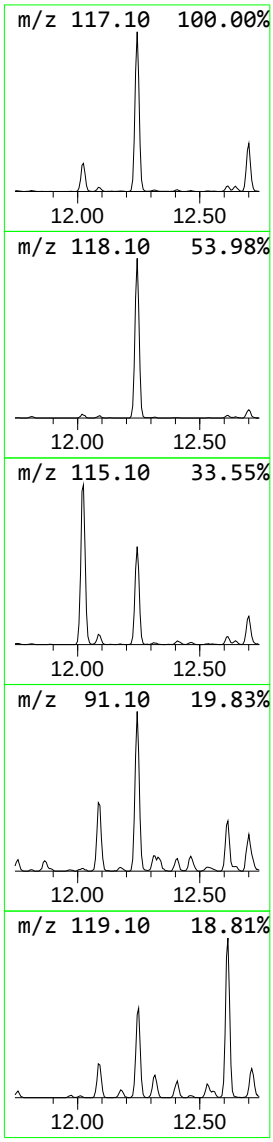
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (Z)-1-Phenylpropene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	32.17 ug/l	390787	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	76
2	Indane	118	C9H10	000496-11-7	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
4	Deltacyclene	118	C9H10	007785-10-6	53
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX113022\
Data File : VX033140.D
Acq On : 30 Nov 2022 18:24
Operator : JC/MD
Sample : N5815-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.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
Butane	1.374	39.3	ug/l	303436	1	5.556	386427	50.0
Butane, 2-methyl-	1.752	142.1	ug/l	1097920	1	5.556	386427	50.0
Pentane	1.959	16.8	ug/l	129983	1	5.556	386427	50.0
Butane, 2,3-dim...	2.782	24.3	ug/l	188094	1	5.556	386427	50.0
1-Pentene	2.867	21.6	ug/l	166988	1	5.556	386427	50.0
Pentane, 3-methyl-	3.105	23.0	ug/l	177947	1	5.556	386427	50.0
Cyclopentane, m...	4.306	52.7	ug/l	407592	1	5.556	386427	50.0
Benzene, 1-ethy...	11.616	18.2	ug/l	220980	4	12.024	607450	50.0
Benzene, 1,2,3-...	12.085	20.3	ug/l	246486	4	12.024	607450	50.0
(Z)-1-Phenylpro...	12.243	32.2	ug/l	390787	4	12.024	607450	50.0