LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

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\82X022322W.M
Title : SW846 8260

Signal : TIC: VX027226.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	27	30	38	rVB	27447	25837	2.32%	0.378%
2	1.374	42	47	52	rBV	55761	51642	4.63%	0.755%
3	1.752	104	109	119	rVB	78631	105643	9.47%	1.545%
4	1.959	137	143	151	rVB2	14535	24210	2.17%	0.354%
5	2.221	181	186	193	rVB	10820	17710	1.59%	0.259%
6	2.788	263	279	283	rBV3	10954	32494	2.91%	0.475%
7	2.874	283	293	300	rVV2	36623	85566	7.67%	1.252%
8	2.959	300	307	318	rVB	109886	231781	20.77%	3.390%
9	3.117	324	333	347	rVB2	34693	87478	7.84%	1.280%
10	3.764	426	439	446	rBV3	6713	24443	2.19%	0.358%
11	3.837	446	451	459	rVB3	4587	11161	1.00%	0.163%
12	4.312	520	529	541	rVB2	22761	65662	5.88%	0.960%
13	5.391	693	706	715	rBV	55405	160847	14.41%	2.353%
14	5.477	715	720	725	rVV2	15243	41724	3.74%	0.610%
15	5.556	725	733	757	rVB	95741	284014	25.45%	4.154%
16	5.958	790	799	805	rBV	58266	153132	13.72%	2.240%
17	6.044	805	813	828	rVV	422436	1115950	100.00%	16.323%
18	6.245	828	846	856	rVV9	12217	57283	5.13%	0.838%
19	6.361	856	865	877	rVB8	3852	14883	1.33%	0.218%
20	6.763	921	931	942	rBV	146016	353023	31.63%	5.164%
21	7.373	1022	1031	1042	rVB6	4734	13752	1.23%	0.201%
22	8.110	1145	1152	1154	rBV	6829	12385	1.11%	0.181%
23	8.147	1154	1158	1163	rVB2	11492	18596	1.67%	0.272%
24	8.427	1197	1204	1210	rBV	17344	29427	2.64%	0.430%
25	8.507	1210	1217	1225	rVB4	10078	18333	1.64%	0.268%
26	8.653	1234	1241	1247	rBV	294091	462810	41.47%	6.769%
27	8.720	1247	1252	1258	rVB	38354	57855	5.18%	0.846%
28	8.958	1286	1291	1298	rVB	13317	21850	1.96%	0.320%
29	9.049	1300	1306	1312	rBV2	14076	21581	1.93%	0.316%
30	9.458	1364	1373	1386	rBV3	17531	34800	3.12%	0.509%
31	9.945	1448	1453	1460	rBV	12329	17529	1.57%	0.256%
32	10.055	1465	1471	1482	rVB	302565	411572	36.88%	6.020%
33	10.195	1488	1494	1500	rBV	471581	589829	52.85%	8.627%
34	10.305	1507	1512	1518	rVB	30270	38196	3.42%	0.559%
35	10.640	1562	1567	1574	rVB	125426	162044	14.52%	2.370%
36	10.964	1614	1620	1625	rVB	46223	57219	5.13%	0.837%

LSC Area Percent Report

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Operator : JC/MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Title : SW846 8260

37	11.079	1634	1639	1649	rBV	246655	316884	28.40%	4.635%
38	11.305	1667	1676	1684	rBV	66292	80964	7.26%	1.184%
39	11.610	1722	1726	1734	rVB	76008	98305	8.81%	1.438%
40	11.756	1745	1750	1756	rVB	138675	177748	15.93%	2.600%
41	12.024	1789	1794	1799	rBV	316215	392501	35.17%	5.741%
42	12.091	1800	1805	1809	rVB	12821	15951	1.43%	0.233%
43	12.244	1823	1830	1836	rBV	286809	348888	31.26%	5.103%
44	12.317	1838	1842	1850	rVB2	8807	15583	1.40%	0.228%
45	12.408	1853	1857	1862	rBV2	17432	24320	2.18%	0.356%
46	12.463	1862	1866	1872	rVB	18163	21570	1.93%	0.315%
47	12.530	1872	1877	1880	rBV	13410	16785	1.50%	0.246%
48	12.616	1887	1891	1894	rBV	27023	33008	2.96%	0.483%
49	12.646	1894	1896	1900	rVB	14255	14637	1.31%	0.214%
50	12.701	1900	1905	1913	rBV	51789	67625	6.06%	0.989%
51	12.921	1935	1941	1945	rBV	30041	38176	3.42%	0.558%
52	12.963	1945	1948	1954	rVV	32943	37763	3.38%	0.552%
53	13.170	1978	1982	1991	rVB	20285	25712	2.30%	0.376%
54	13.292	1998	2002	2007	rVB2	35343	45591	4.09%	0.667%
55	13.427	2019	2024	2028	rVB	16694	21350	1.91%	0.312%
56	13.664	2061	2063	2069	rVB2	8876	11507	1.03%	0.168%
57	13.774	2074	2081	2089	rBV	58624	75433	6.76%	1.103%
58	13.865	2090	2096	2101	rVB2	8180	13506	1.21%	0.198%
59	14.780	2242	2246	2251	rBV	23504	30802	2.76%	0.451%

Sum of corrected areas: 6836870

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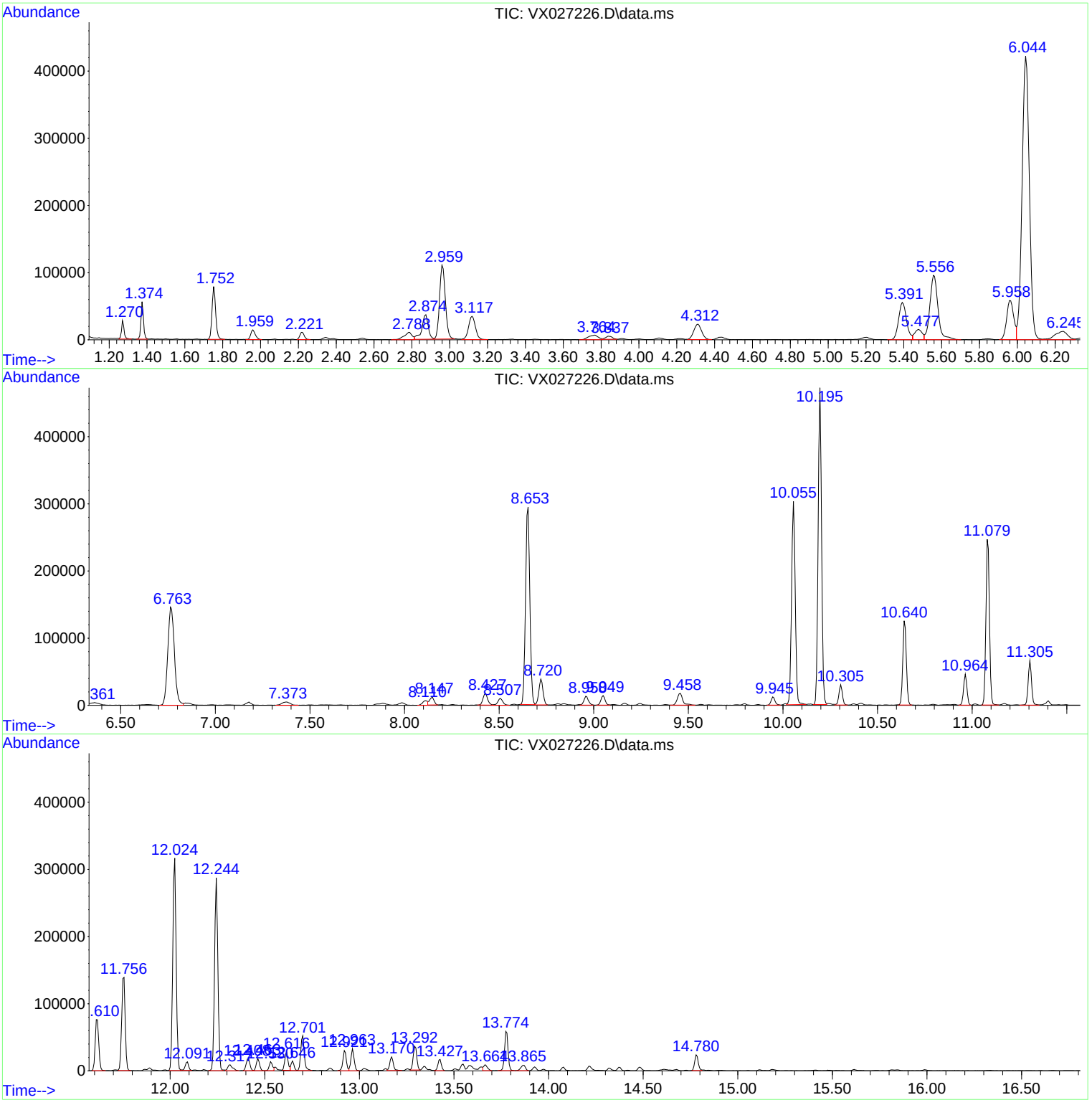
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

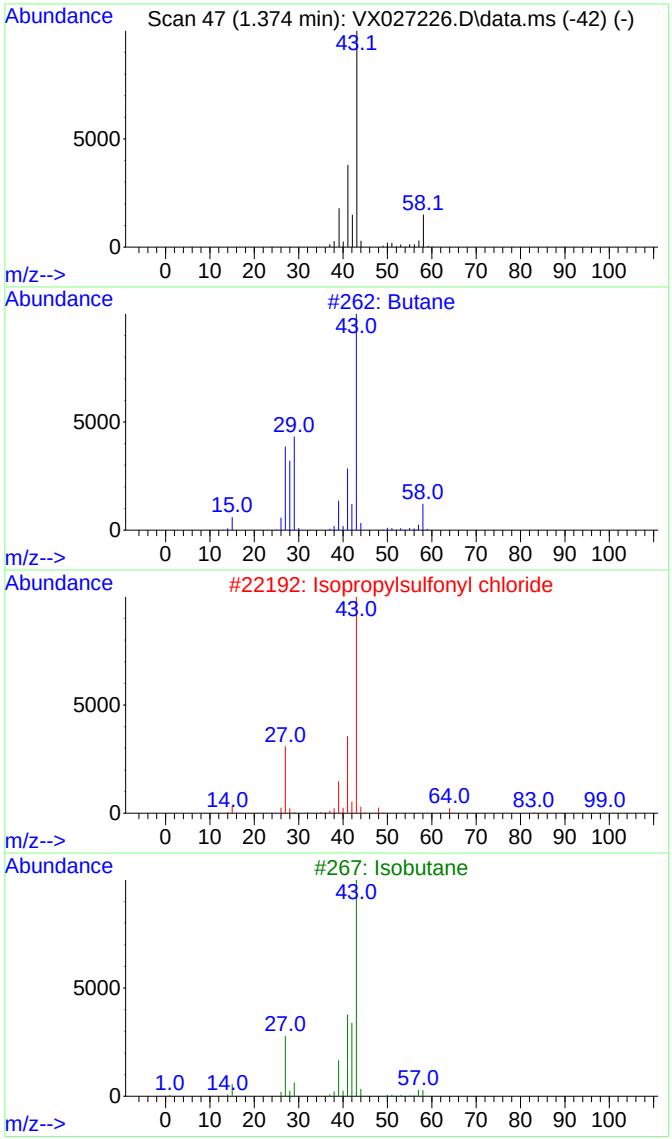
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

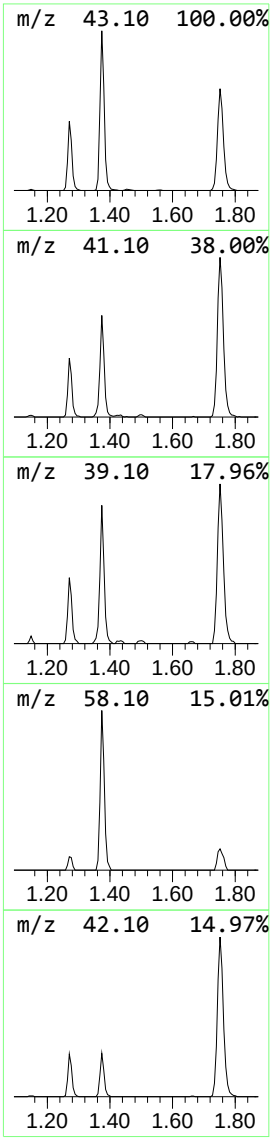
****

Peak Number 1 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.374	9.09 ug/l	51642	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
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	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

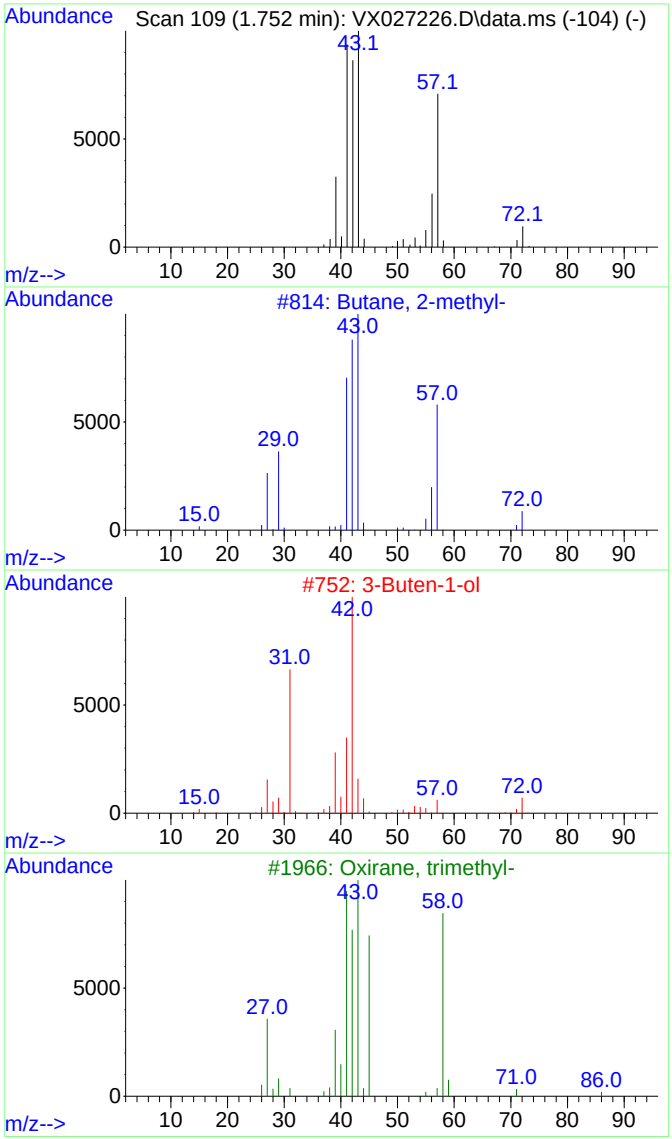
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

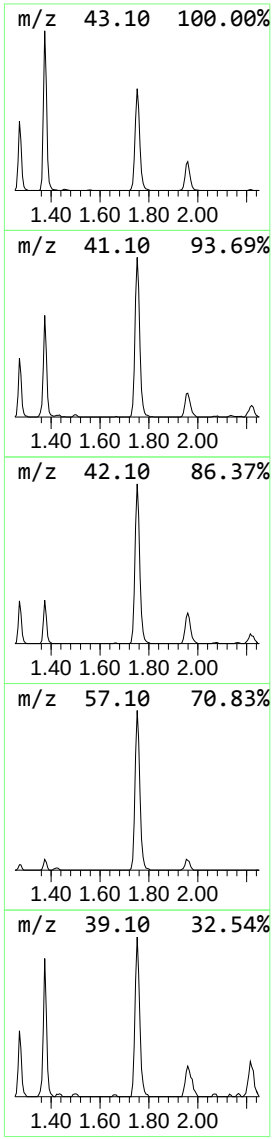
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	18.60 ug/l	105643	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4	Pentane	72	C5H12	000109-66-0	33
5	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

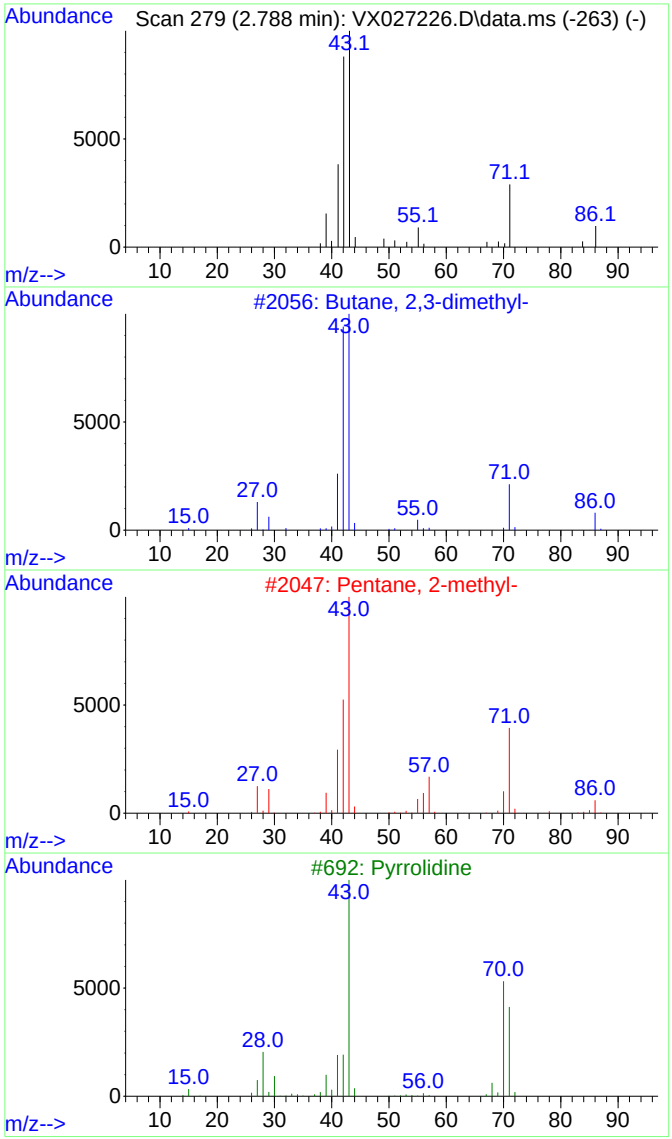
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

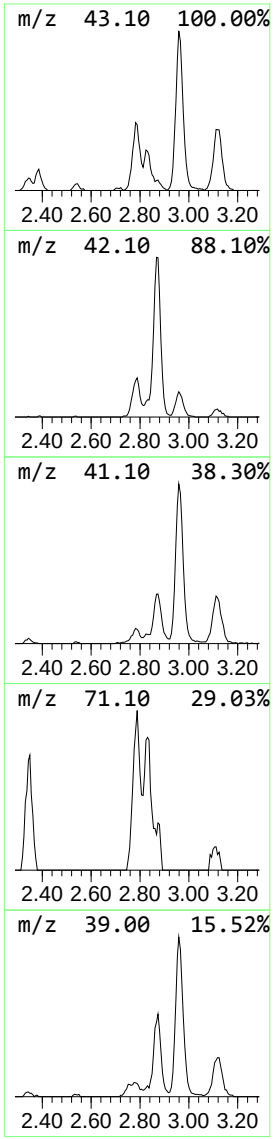
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.788	5.72 ug/l	32494	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Pyrrolidine	71	C4H9N	000123-75-1	12
4	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	9
5	Butane, 2-methyl-	72	C5H12	000078-78-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

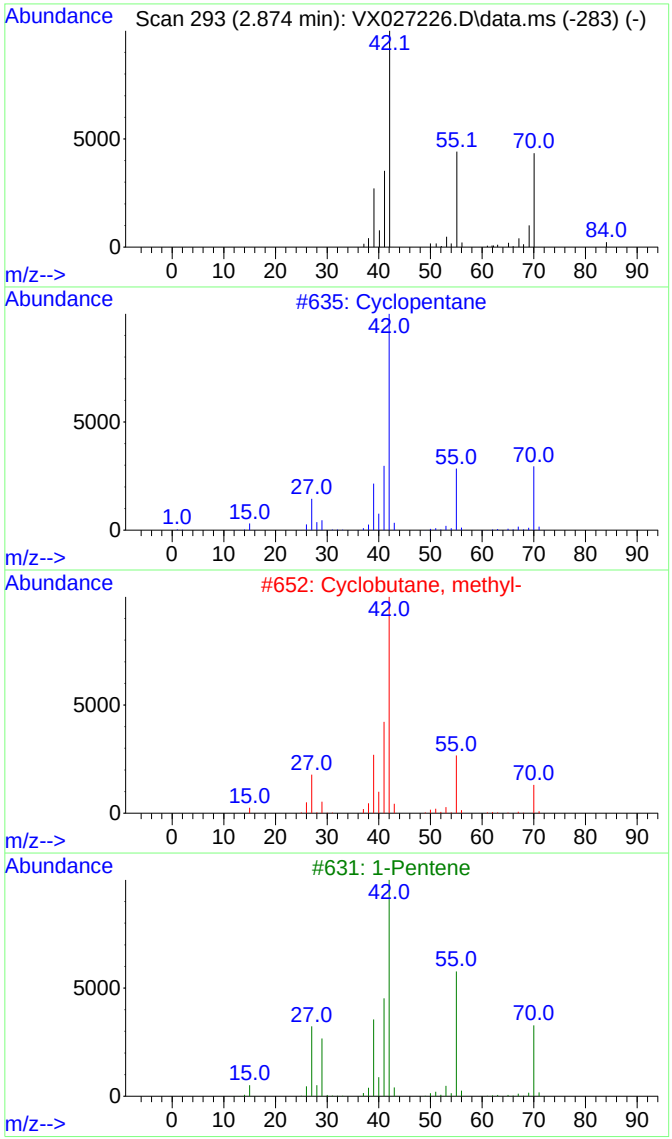
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

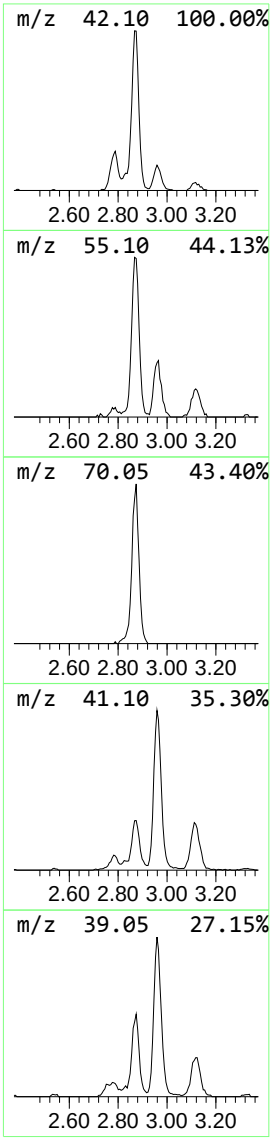
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.874	15.06 ug/l	85566	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	1-Pentene	70	C5H10	000109-67-1	59
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	32
5	1-Pentanol	88	C5H12O	000071-41-0	9





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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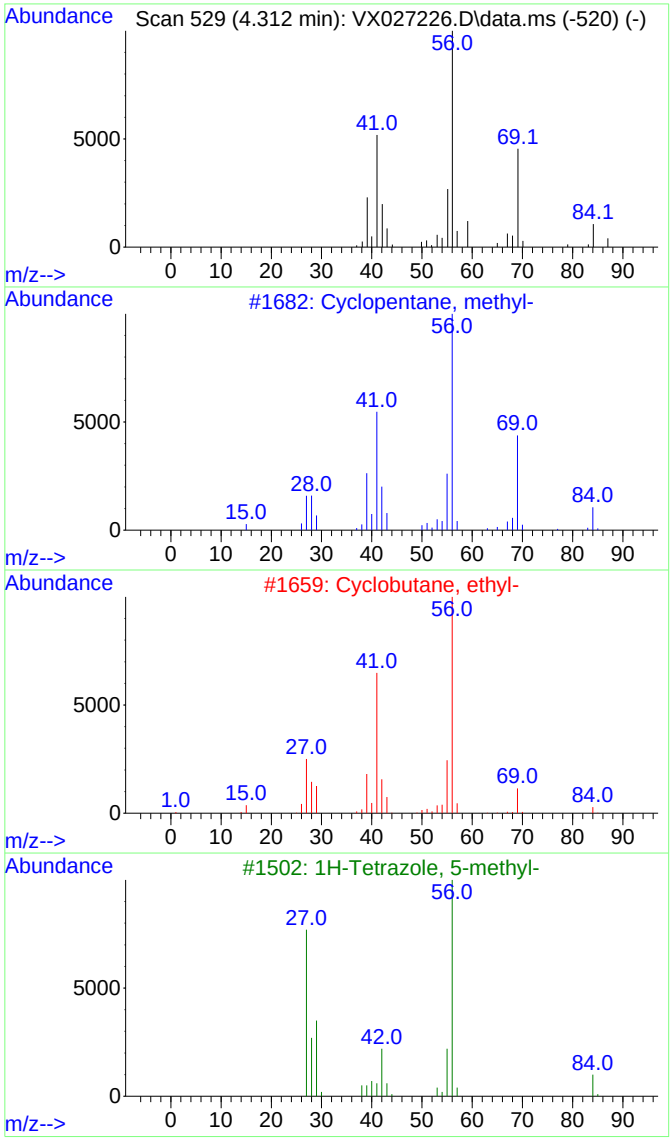
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

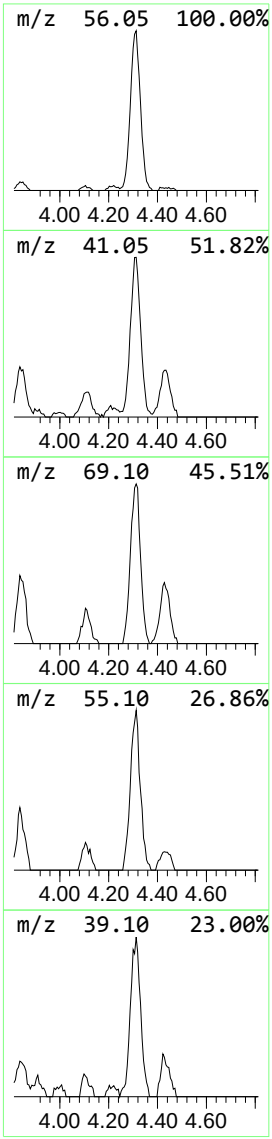
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	11.56 ug/l	65662	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	93
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	42





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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

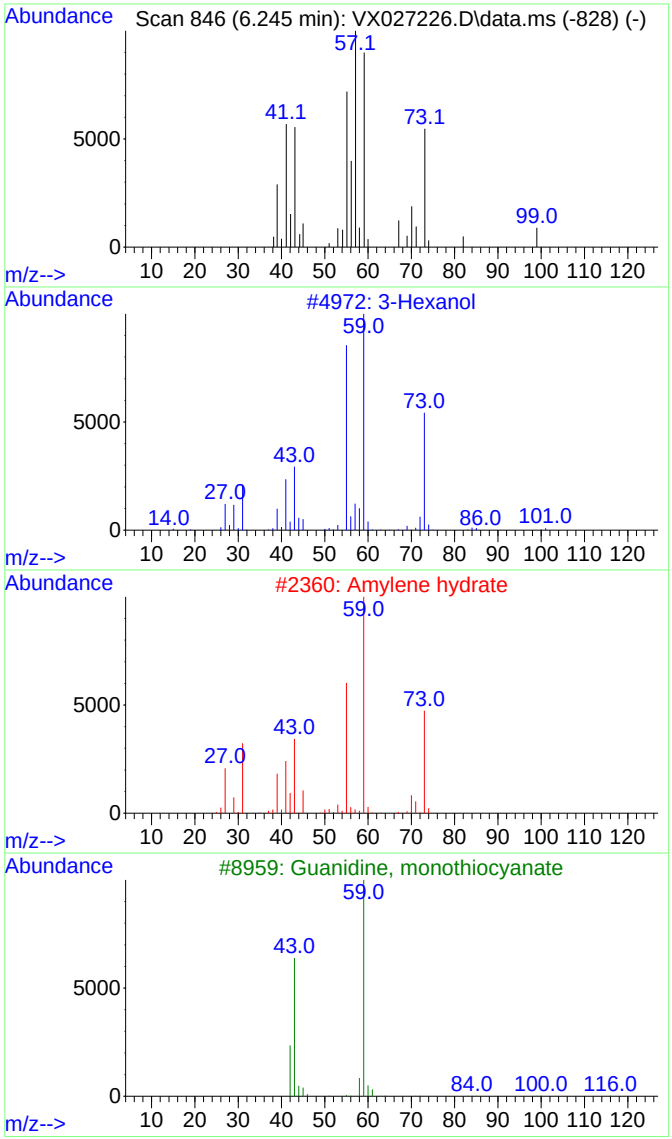
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

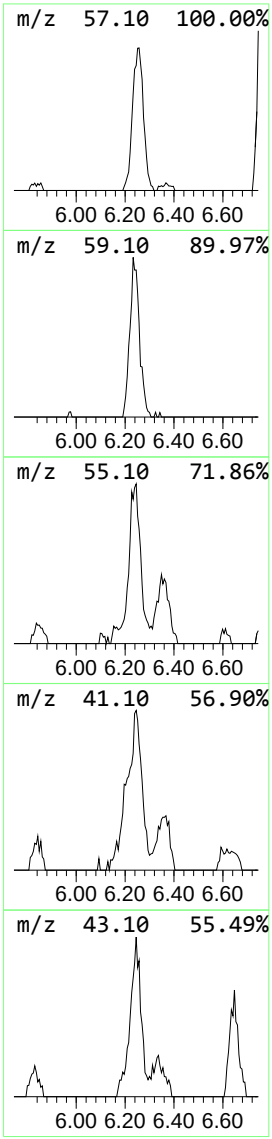
****

Peak Number 6 unknown6.245 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	8.11 ug/l	57283	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanol	102	C6H14O	000623-37-0	47
2	Amylene hydrate	88	C5H12O	000075-85-4	37
3	Guanidine, monothiocyanate	116	C2H4N4S	056960-89-5	35
4	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	32
5	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	16





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

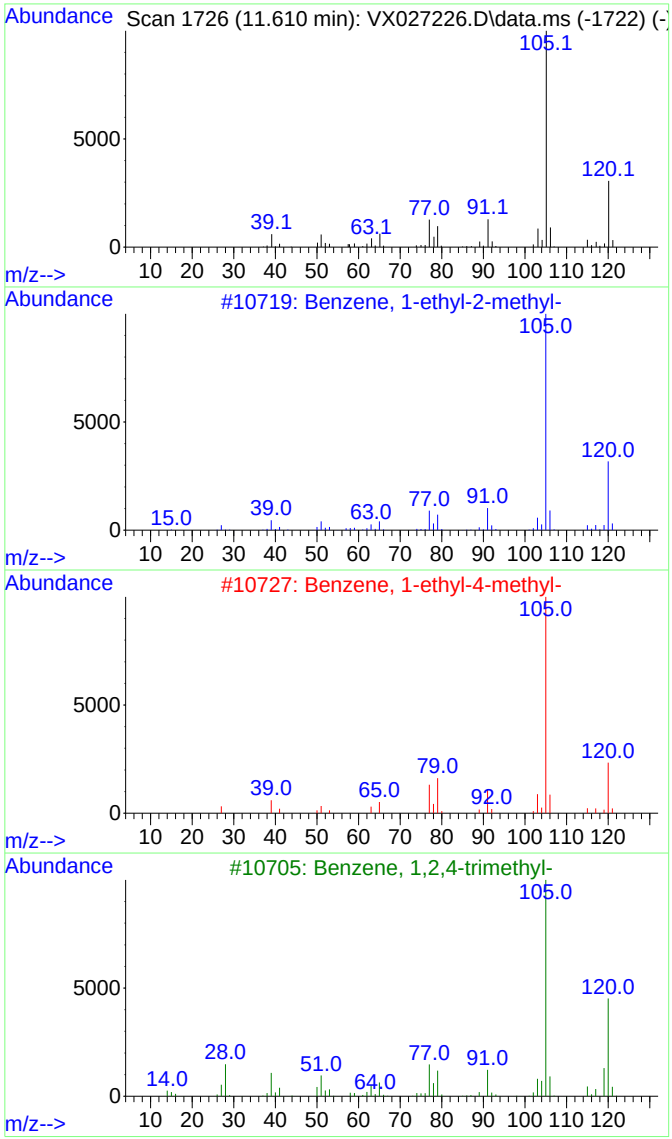
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

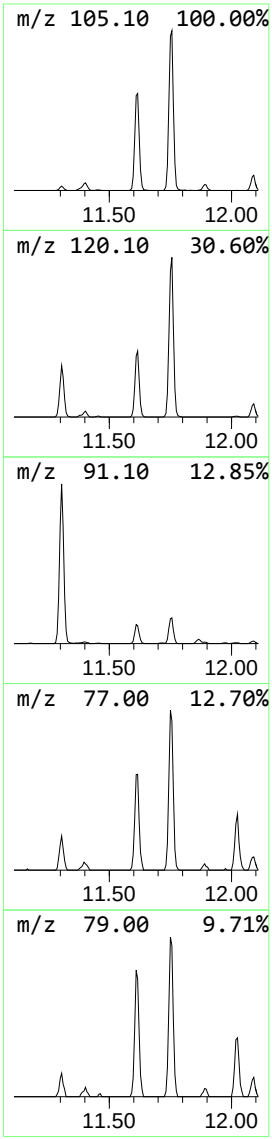
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.610	12.52 ug/l	98305	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	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

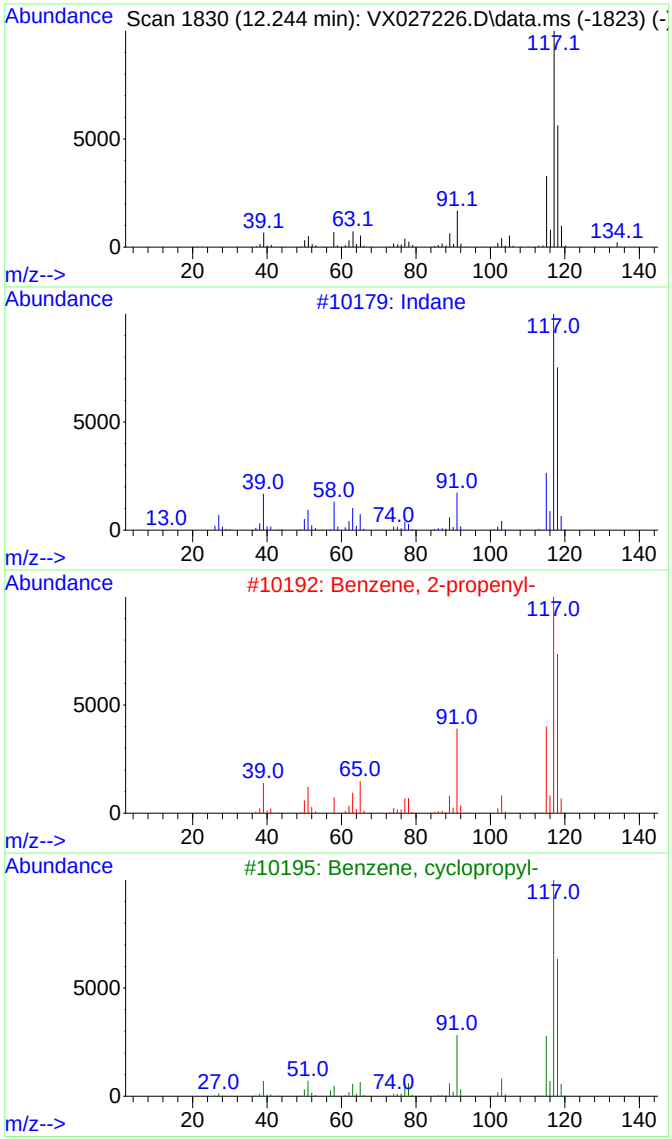
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

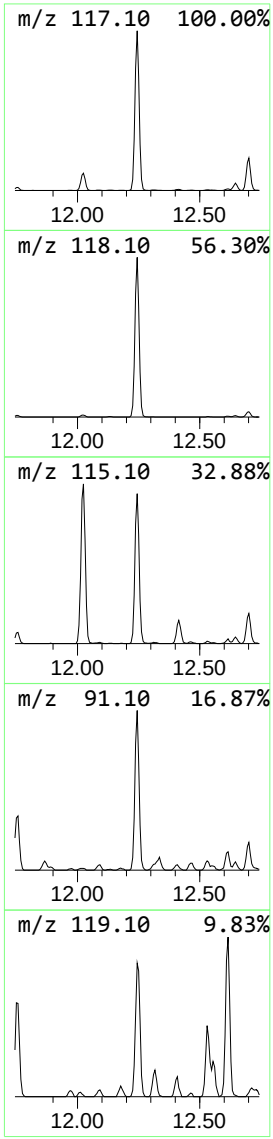
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	44.44 ug/l	348888	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53





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Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

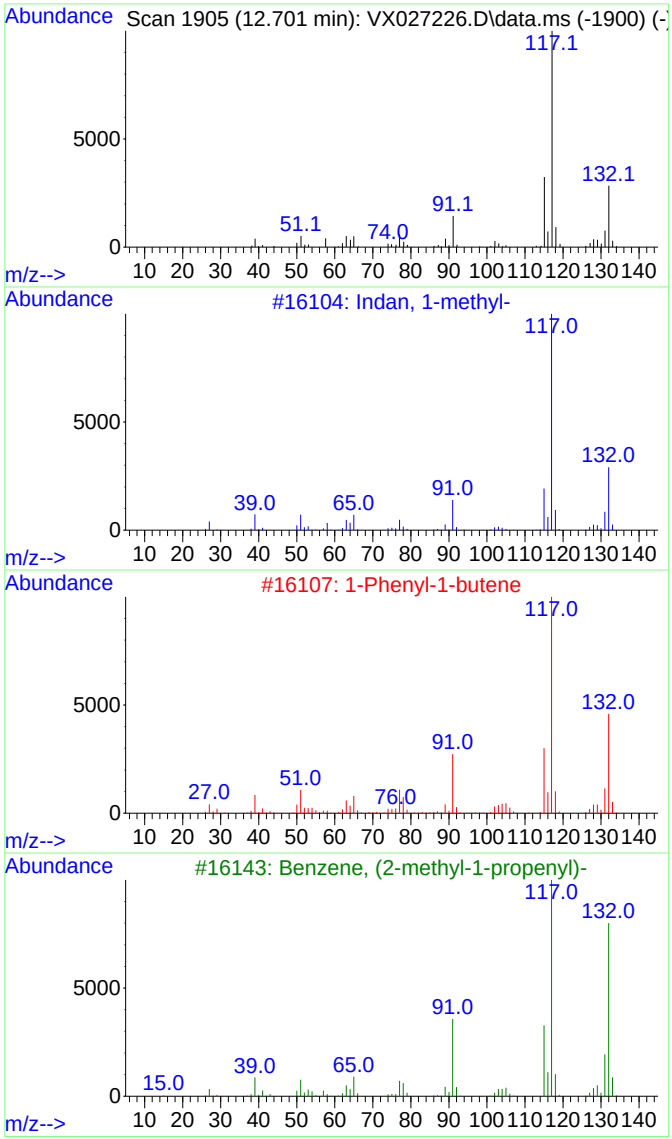
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

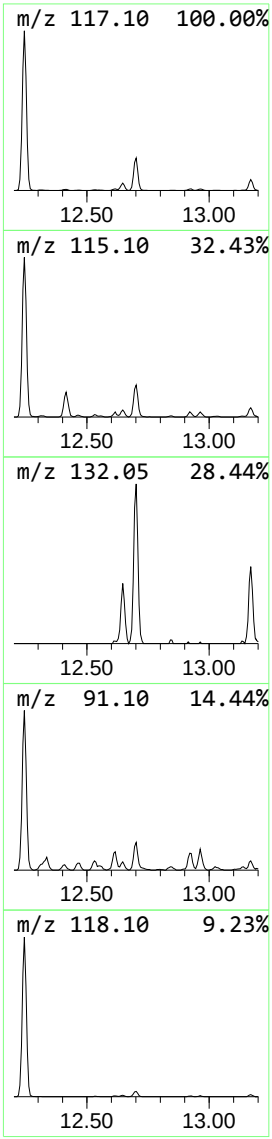
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Indan, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	8.61 ug/l	67625	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	90
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	83
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

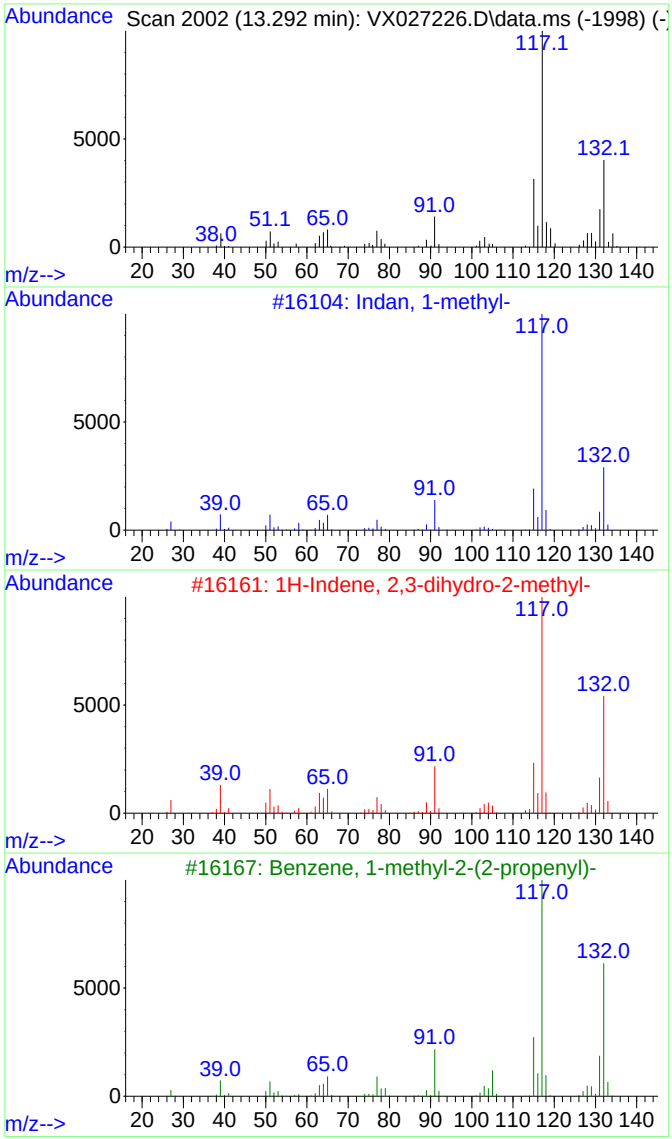
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.M
Quant Title : SW846 8260

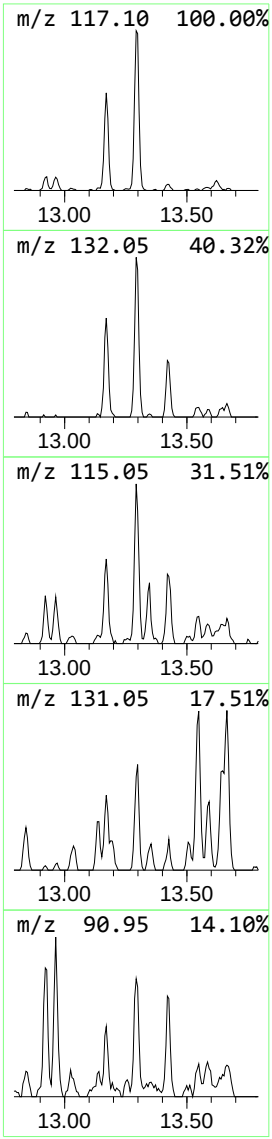
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1H-Indene, 2,3-dihydro-2-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	5.81 ug/l	45591	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	87
2	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	87
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
4	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5	1-Phenyl-1-butene	132	C10H12	000824-90-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022822\
Data File : VX027226.D
Acq On : 28 Feb 2022 17:36
Operator : JC/MD
Sample : N1688-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022322W.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	9.1	ug/l	51642	1	5.556	284014	50.0
Butane, 2-methyl-	1.752	18.6	ug/l	105643	1	5.556	284014	50.0
Butane, 2,3-dim...	2.788	5.7	ug/l	32494	1	5.556	284014	50.0
Cyclopentane	2.874	15.1	ug/l	85566	1	5.556	284014	50.0
Cyclopentane, m...	4.312	11.6	ug/l	65662	1	5.556	284014	50.0
unknown6.245	6.245	8.1	ug/l	57283	2	6.763	353023	50.0
Benzene, 1-ethy...	11.610	12.5	ug/l	98305	4	12.024	392501	50.0
Indane	12.244	44.4	ug/l	348888	4	12.024	392501	50.0
Indan, 1-methyl-	12.701	8.6	ug/l	67625	4	12.024	392501	50.0
1H-Indene, 2,3-...	13.292	5.8	ug/l	45591	4	12.024	392501	50.0