LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021825\
Data File : VX044992.D
Acq On : 18 Feb 2025 16:54
Operator : JC/MD
Sample : Q1376-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW32

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\82X021025W.M
Title : SW846 8260

Signal : TIC: VX044992.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	22	rVB3	61666	78191	2.23%	0.211%
2	1.264	26	29	40	rBV	648978	878958	25.05%	2.369%
3	1.368	43	46	65	rVB	2521938	2907704	82.87%	7.837%
4	1.733	101	106	125	rVB	2362650	3444074	98.16%	9.282%
5	1.947	136	141	156	rVB2	236280	412260	11.75%	1.111%
6	2.209	177	184	196	rVB	574826	872899	24.88%	2.353%
7	2.331	198	204	210	rBV	42327	82337	2.35%	0.222%
8	2.776	261	277	280	rBV2	135998	394804	11.25%	1.064%
9	2.861	280	291	302	rVV	957576	2262900	64.49%	6.099%
10	2.959	302	307	318	rVV	18105	45716	1.30%	0.123%
11	3.093	320	329	342	rVB	209091	483487	13.78%	1.303%
12	3.727	423	433	441	rBV	52656	130382	3.72%	0.351%
13	3.831	442	450	457	rBV	35396	86604	2.47%	0.233%
14	4.093	479	493	504	rVB2	59424	171664	4.89%	0.463%
15	4.202	504	511	516	rVV	18355	48847	1.39%	0.132%
16	4.294	516	526	538	rVV	607620	1747269	49.80%	4.709%
17	4.416	538	546	562	rVB2	51485	165049	4.70%	0.445%
18	5.184	650	672	689	rVB2	102483	355639	10.14%	0.959%
19	5.379	694	704	709	rBV2	70973	203667	5.80%	0.549%
20	5.464	709	718	726	rVV	476637	1505235	42.90%	4.057%
21	5.544	726	731	737	rVV	98772	284215	8.10%	0.766%
22	5.611	738	742	760	rVB3	63755	189820	5.41%	0.512%
23	5.830	766	778	790	rBV4	54314	187308	5.34%	0.505%
24	5.946	790	797	802	rVV	77140	193671	5.52%	0.522%
25	6.031	802	811	823	rVV	1290760	3508762	100.00%	9.457%
26	6.153	823	831	841	rVV3	120485	517601	14.75%	1.395%
27	6.251	841	847	855	rVV4	126991	367158	10.46%	0.990%
28	6.348	855	863	876	rVB2	88573	255940	7.29%	0.690%
29	6.476	876	884	898	rBV3	28525	81008	2.31%	0.218%
30	6.757	920	930	940	rBV	174778	472727	13.47%	1.274%
31	6.848	942	945	957	rVB4	25743	59662	1.70%	0.161%
32	7.165	989	997	1004	rBV	32683	75420	2.15%	0.203%
33	7.373	1019	1031	1042	rVB2	244360	638681	18.20%	1.721%
34	7.488	1042	1050	1056	rBV2	20009	49706	1.42%	0.134%
35	7.653	1071	1077	1088	rVB	33394	66553	1.90%	0.179%
36	7.769	1088	1096	1103	rBV	72495	147211	4.20%	0.397%

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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
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Title : SW846 8260

37	7.879	1103	1114	1120	rBV4	24678	71529	2.04%	0.193%
38	7.952	1120	1126	1143	rVB3	53708	156064	4.45%	0.421%
39	8.104	1143	1151	1153	rBV	27491	54125	1.54%	0.146%
40	8.141	1153	1157	1161	rVB	32089	50181	1.43%	0.135%
41	8.311	1178	1185	1192	rBV3	50293	106381	3.03%	0.287%
42	8.403	1192	1200	1209	rBV2	220056	517911	14.76%	1.396%
43	8.500	1211	1216	1224	rVB3	103628	193455	5.51%	0.521%
44	8.598	1224	1232	1235	rBV3	139634	280898	8.01%	0.757%
45	8.647	1235	1240	1246	rVB	347504	561000	15.99%	1.512%
46	8.714	1246	1251	1256	rBV	283224	420911	12.00%	1.134%
47	8.769	1256	1260	1264	rVV	90066	128487	3.66%	0.346%
48	8.842	1269	1272	1279	rVB3	34418	58836	1.68%	0.159%
49	8.921	1279	1285	1288	rBV3	19263	36381	1.04%	0.098%
50	8.970	1288	1293	1299	rVV	218909	353042	10.06%	0.952%
51	9.049	1302	1306	1310	rVV	62830	107769	3.07%	0.290%
52	9.098	1310	1314	1320	rVB	126731	196524	5.60%	0.530%
53	9.372	1355	1359	1363	rBV	27146	40745	1.16%	0.110%
54	9.451	1363	1372	1376	rVV	162480	292116	8.33%	0.787%
55	9.506	1376	1381	1386	rVV3	76394	136070	3.88%	0.367%
56	9.561	1386	1390	1394	rVB	29936	42711	1.22%	0.115%
57	9.616	1394	1399	1402	rBV	53682	82585	2.35%	0.223%
58	9.829	1430	1434	1446	rVB	43461	76348	2.18%	0.206%
59	9.957	1446	1455	1459	rBV3	122689	250347	7.13%	0.675%
60	10.049	1466	1470	1475	rBV	351921	477955	13.62%	1.288%
61	10.122	1479	1482	1488	rVV	59721	89593	2.55%	0.241%
62	10.189	1488	1493	1503	rVB4	43345	109685	3.13%	0.296%
63	10.299	1503	1511	1517	rBV	418289	611336	17.42%	1.648%
64	10.451	1532	1536	1543	rVB2	45836	81754	2.33%	0.220%
65	10.592	1549	1559	1564	rBV6	70003	195998	5.59%	0.528%
66	10.640	1564	1567	1573	rVB2	53492	81072	2.31%	0.219%
67	10.774	1581	1589	1597	rVB2	77118	142846	4.07%	0.385%
68	10.854	1597	1602	1614	rVV6	55461	127017	3.62%	0.342%
69	10.957	1614	1619	1623	rVV	364673	462475	13.18%	1.246%
70	11.006	1623	1627	1634	rVV4	54799	98071	2.80%	0.264%
71	11.079	1634	1639	1643	rVV	298479	401843	11.45%	1.083%
72	11.122	1643	1646	1650	rVV	50254	71422	2.04%	0.192%
73	11.183	1650	1656	1658	rVV4	21588	39308	1.12%	0.106%
74	11.219	1658	1662	1666	rVV5	46883	78129	2.23%	0.211%
75	11.268	1666	1670	1672	rVV	106826	148959	4.25%	0.401%
76	11.299	1672	1675	1685	rVV	669259	887979	25.31%	2.393%

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77	11.384	1685	1689	1695	rVV4	26935	59764	1.70%	0.161%
78	11.451	1696	1700	1707	rVB	43179	66111	1.88%	0.178%
79	11.610	1721	1726	1734	rVB	139974	186921	5.33%	0.504%
80	11.860	1761	1767	1769	rBV2	34037	53995	1.54%	0.146%
81	11.884	1769	1771	1782	rVB3	50465	83718	2.39%	0.226%
82	12.018	1787	1793	1799	rBV	413448	526852	15.02%	1.420%
83	12.085	1799	1804	1814	rBV	360220	455564	12.98%	1.228%
84	12.238	1824	1829	1835	rBV	1552254	1975098	56.29%	5.323%
85	12.311	1837	1841	1850	rVB3	63828	129618	3.69%	0.349%
86	12.402	1850	1856	1862	rBV	25761	43117	1.23%	0.116%
87	12.609	1886	1890	1893	rBV	86246	98071	2.80%	0.264%
88	12.640	1893	1895	1900	rVV2	47780	69189	1.97%	0.186%
89	12.695	1900	1904	1912	rVB	199211	265314	7.56%	0.715%
90	12.811	1918	1923	1926	rBV	26918	43171	1.23%	0.116%
91	12.920	1933	1941	1945	rBV	145475	209112	5.96%	0.564%
92	12.963	1945	1948	1954	rVV3	25040	47153	1.34%	0.127%
93	13.024	1954	1958	1964	rVB3	43245	66515	1.90%	0.179%
94	13.164	1978	1981	1990	rVB	174782	232517	6.63%	0.627%
95	13.286	1997	2001	2006	rVB2	242349	313963	8.95%	0.846%
96	13.420	2016	2023	2029	rVB4	31793	67753	1.93%	0.183%
97	13.579	2046	2049	2052	rVB2	46358	56860	1.62%	0.153%
98	13.664	2060	2063	2070	rVB3	32901	52206	1.49%	0.141%
99	13.774	2071	2081	2090	rBV	160601	231002	6.58%	0.623%
100	14.780	2239	2246	2252	rBV2	52883	76636	2.18%	0.207%

Sum of corrected areas: 37103207

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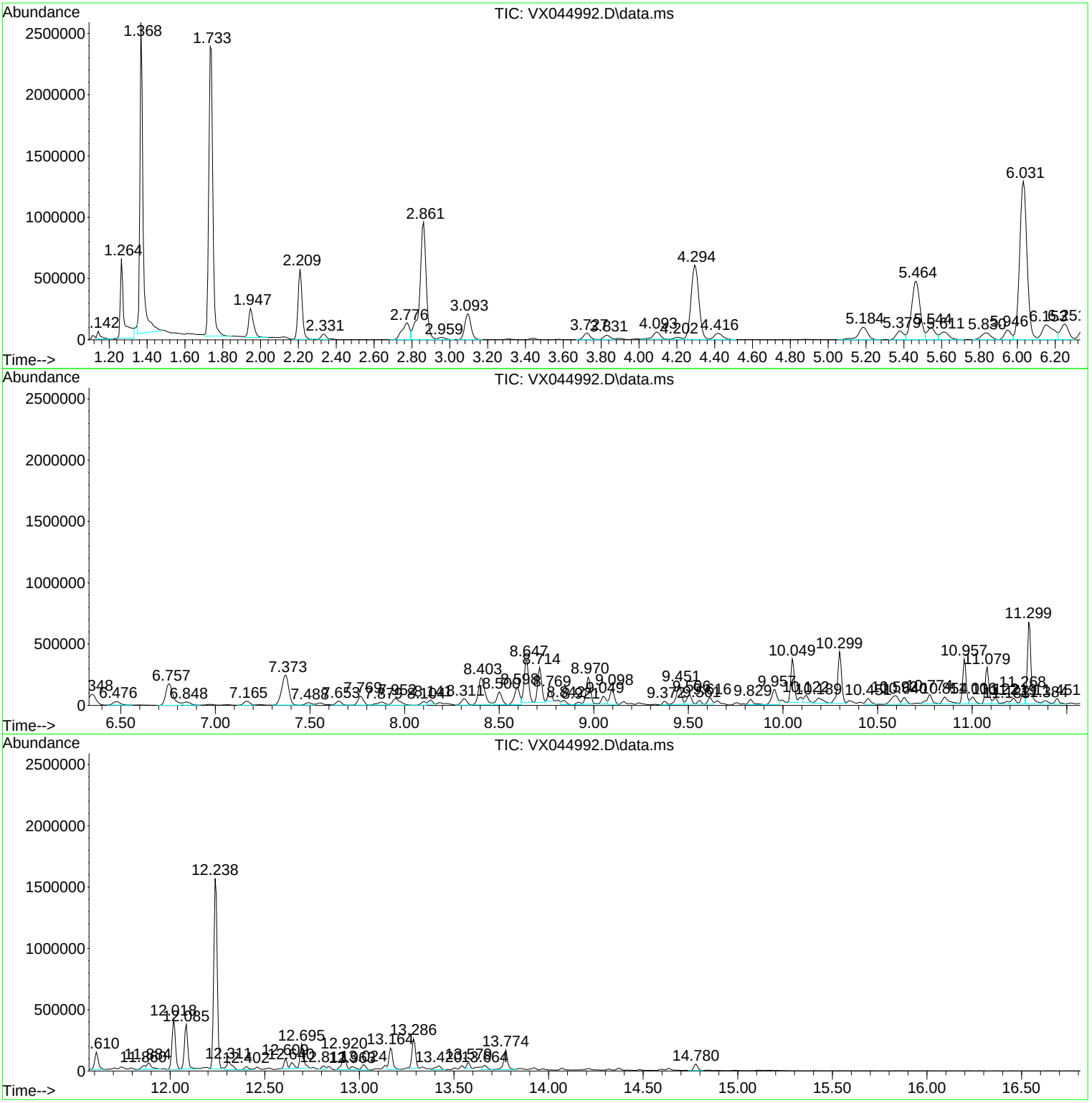
Instrument :
MSVOA_X
ClientSampleId :
MW32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

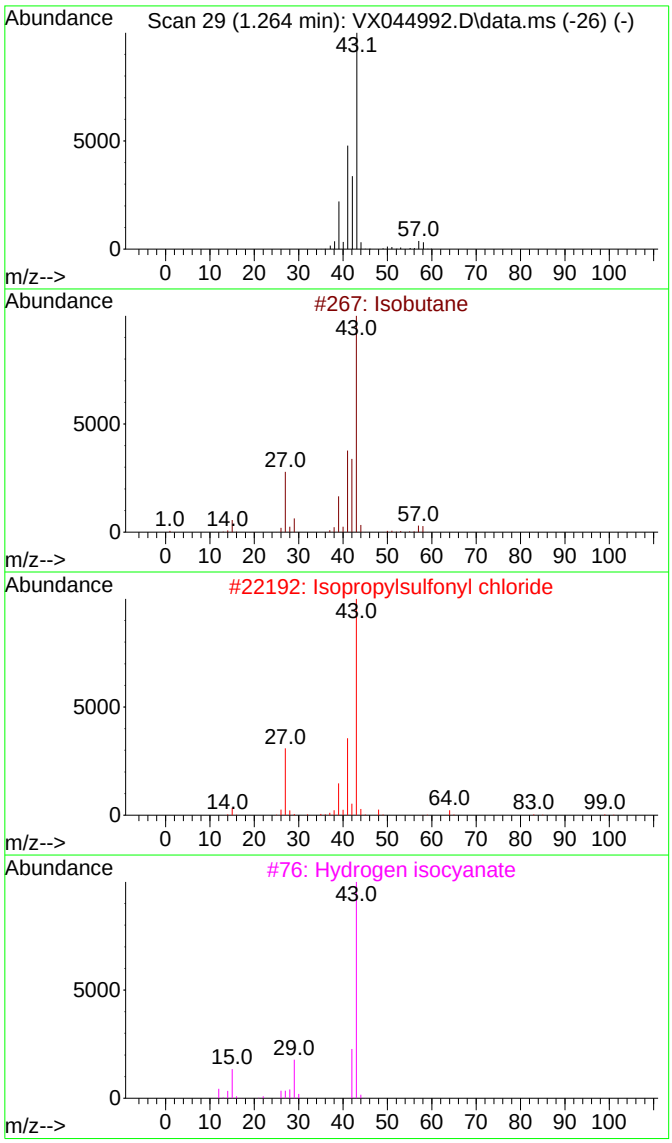
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

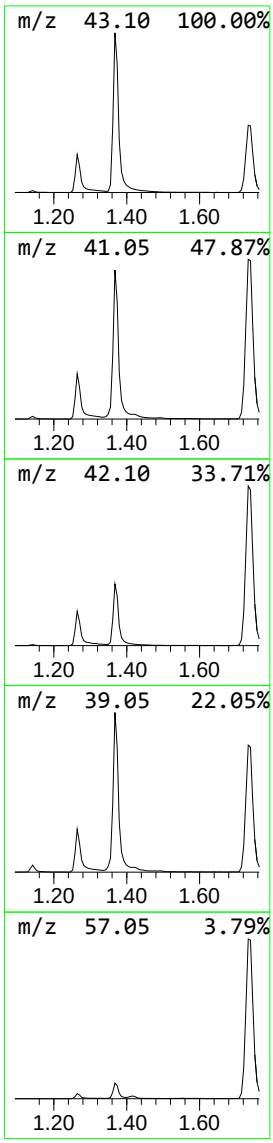
****

Peak Number 1 Isobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	154.63 ug/l	878958	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	80
2	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
3	Hydrogen isocyanate	43	CHNO	000075-13-8	4
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
5	Cyclobutylamine	71	C4H9N	002516-34-9	4





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

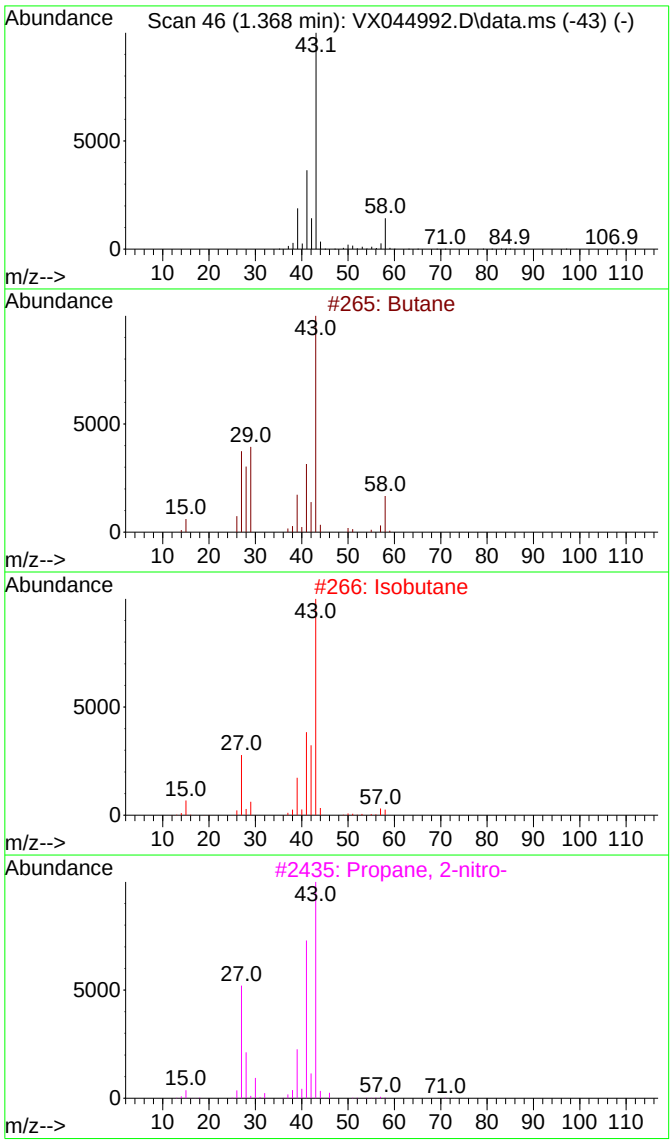
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

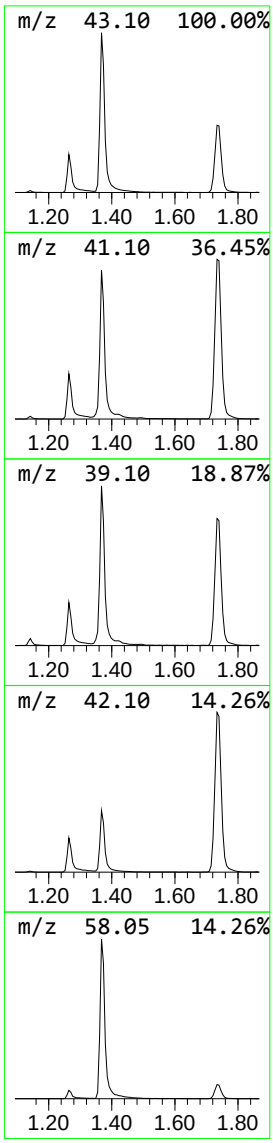
****

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	511.53 ug/l	2907700	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Isobutane	58	C4H10	000075-28-5	9
3	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





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MSVOA_X
ClientSampleId :
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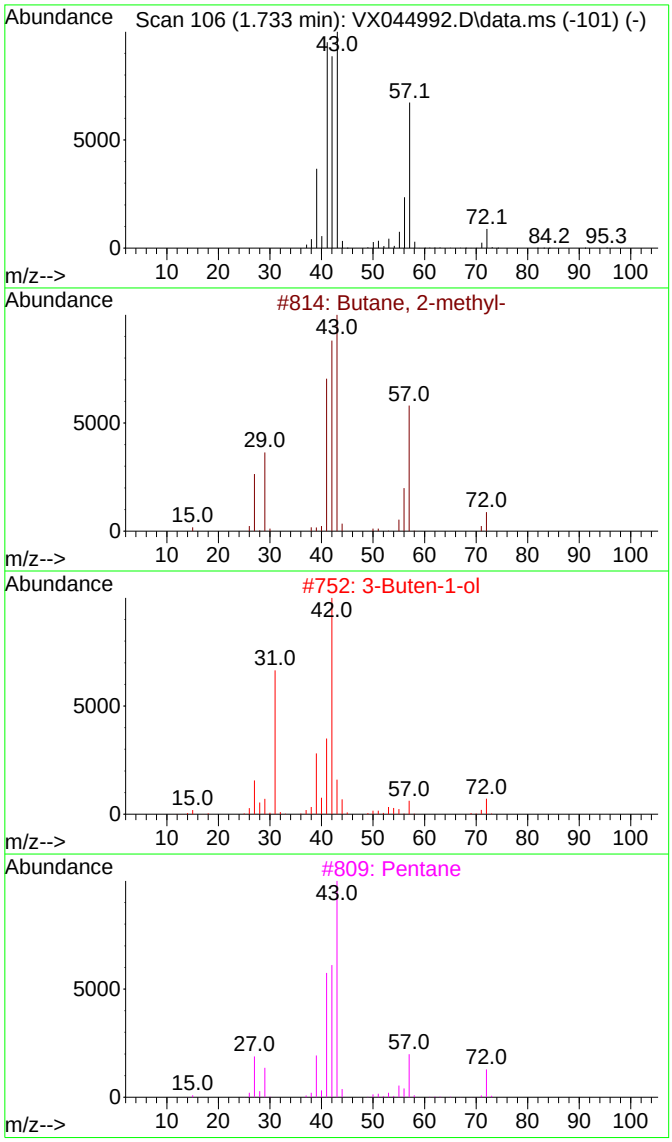
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

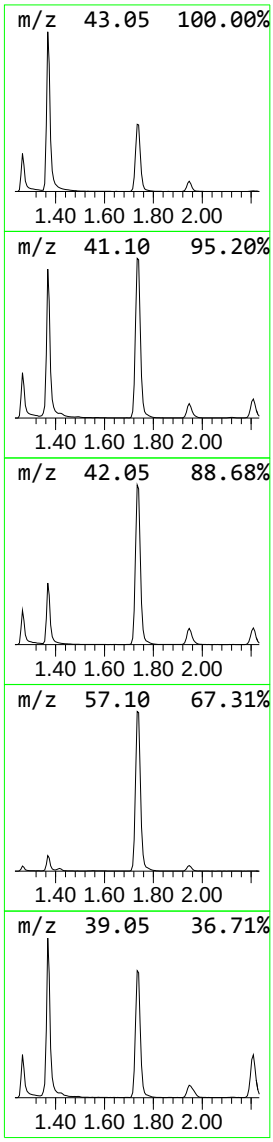
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.733	605.89 ug/l	3444070	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5	Azetidine	57	C3H7N	000503-29-7	9





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Quant Title : SW846 8260

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

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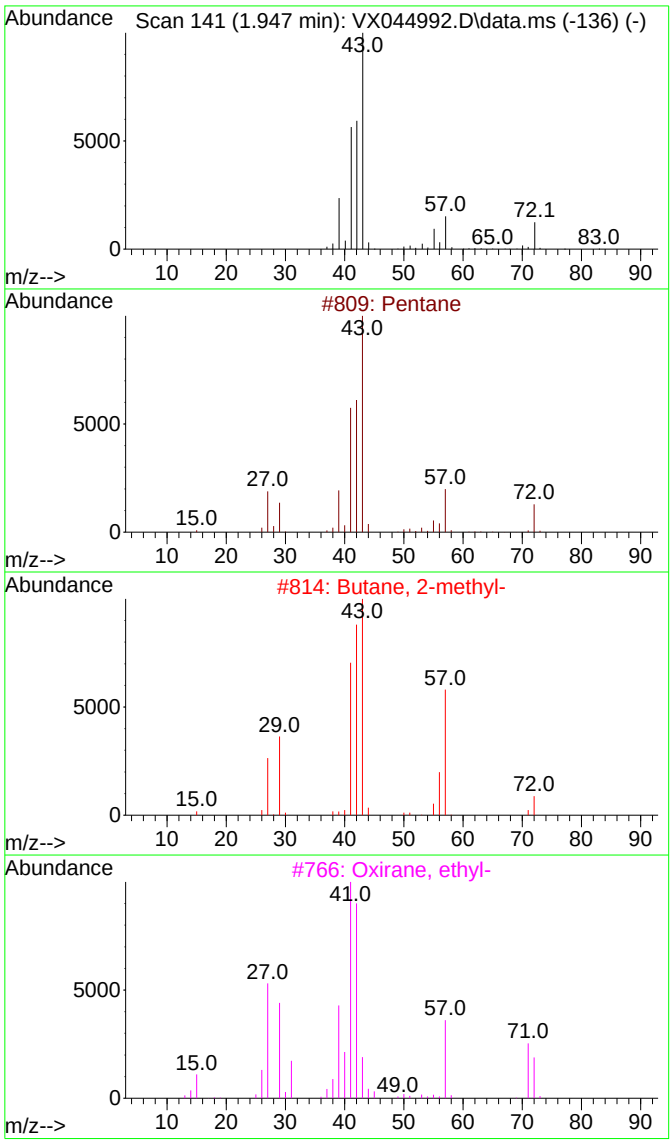
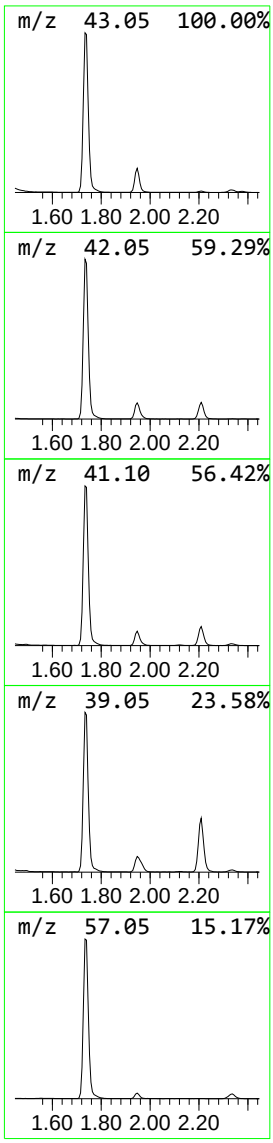
Peak Number 4 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.947	72.53 ug/l	412260	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	87
2	Butane, 2-methyl-	72	C5H12	000078-78-4	59
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	43
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	10





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW32

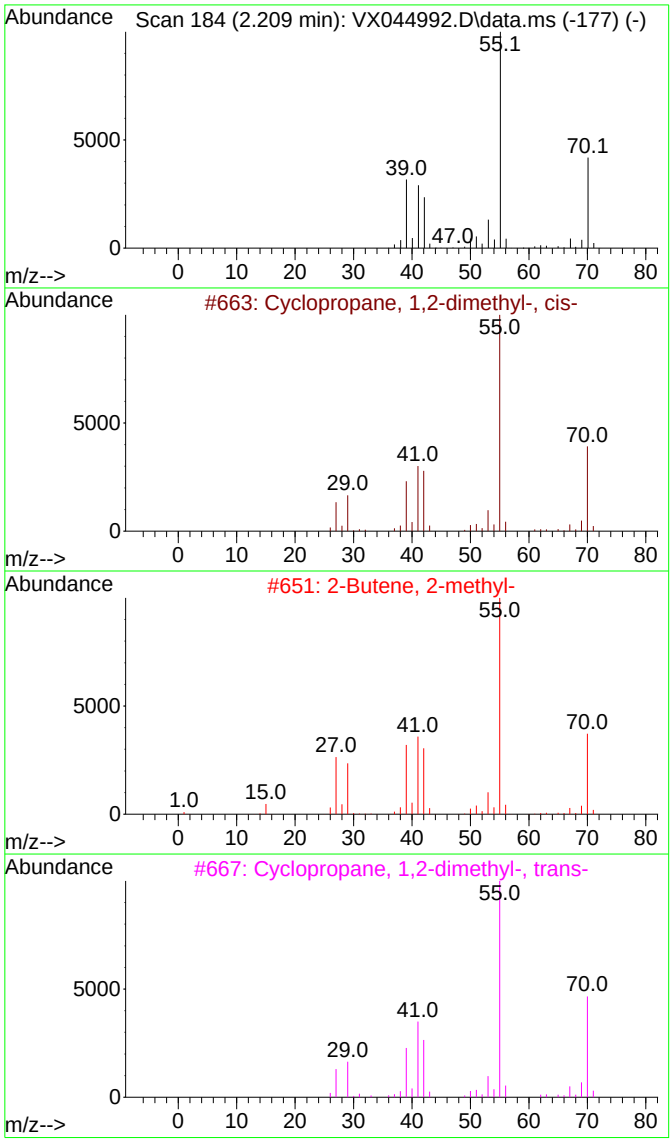
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

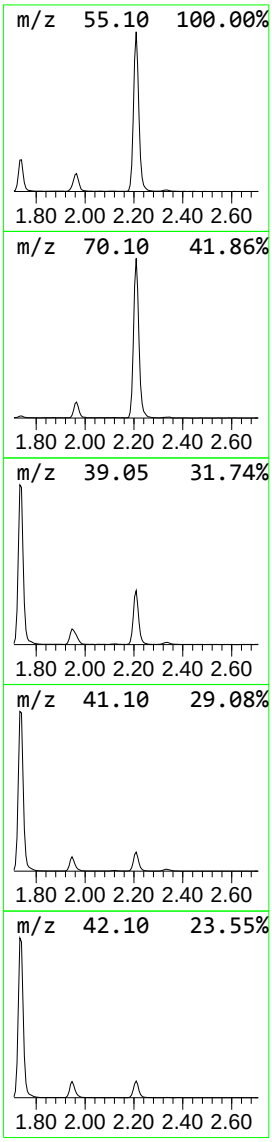
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.209	153.56 ug/l	872899	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
4	2-Pentene, (E)-	70	C5H10	000646-04-8	87
5	2-Pentene	70	C5H10	000109-68-2	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021825\
Data File : VX044992.D
Acq On : 18 Feb 2025 16:54
Operator : JC/MD
Sample : Q1376-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW32

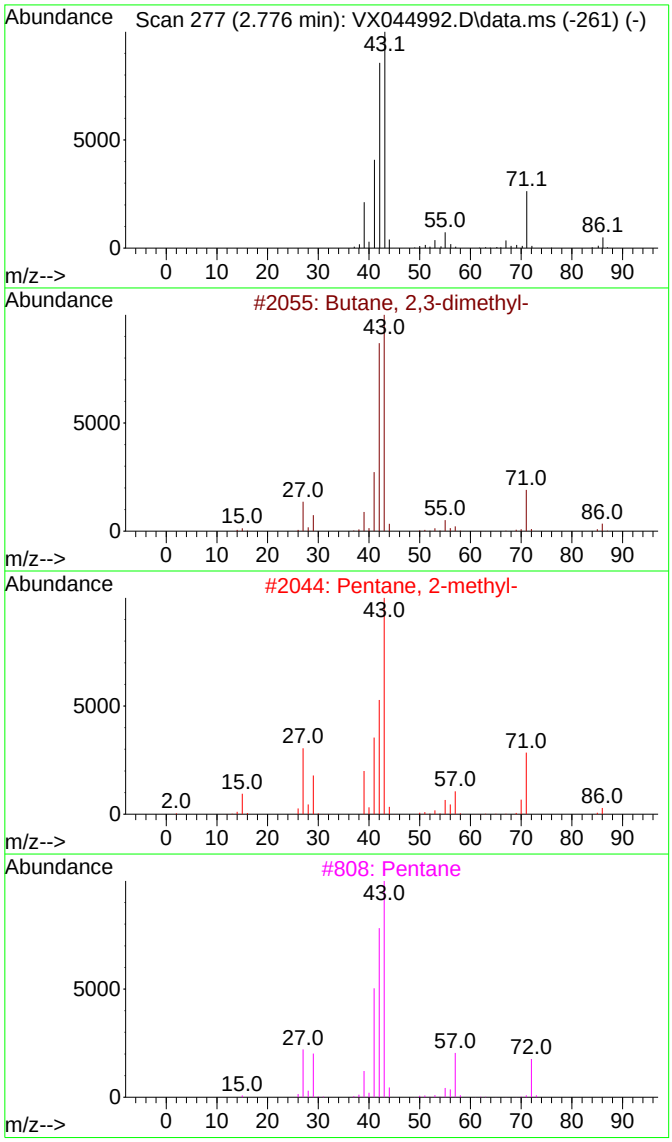
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

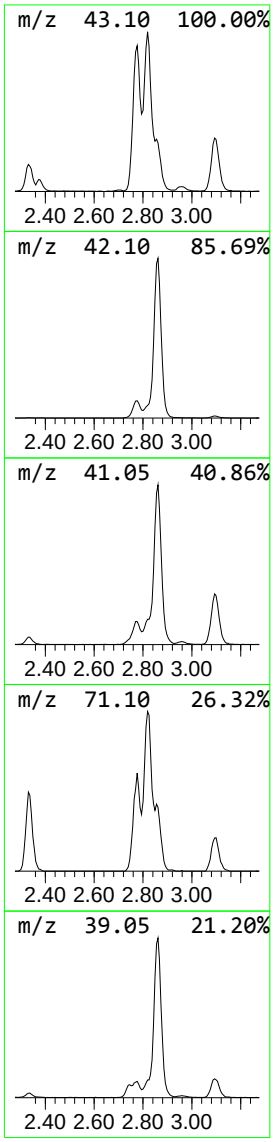
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.776	69.46 ug/l	394804	Pentafluorobenzene	5.544

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	47
3	Pentane	72	C5H12	000109-66-0	42
4	Tetrahydrofuran	72	C4H8O	000109-99-9	36
5	Cyclobutane, methyl-	70	C5H10	000598-61-8	28





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Data File : VX044992.D
Acq On : 18 Feb 2025 16:54
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

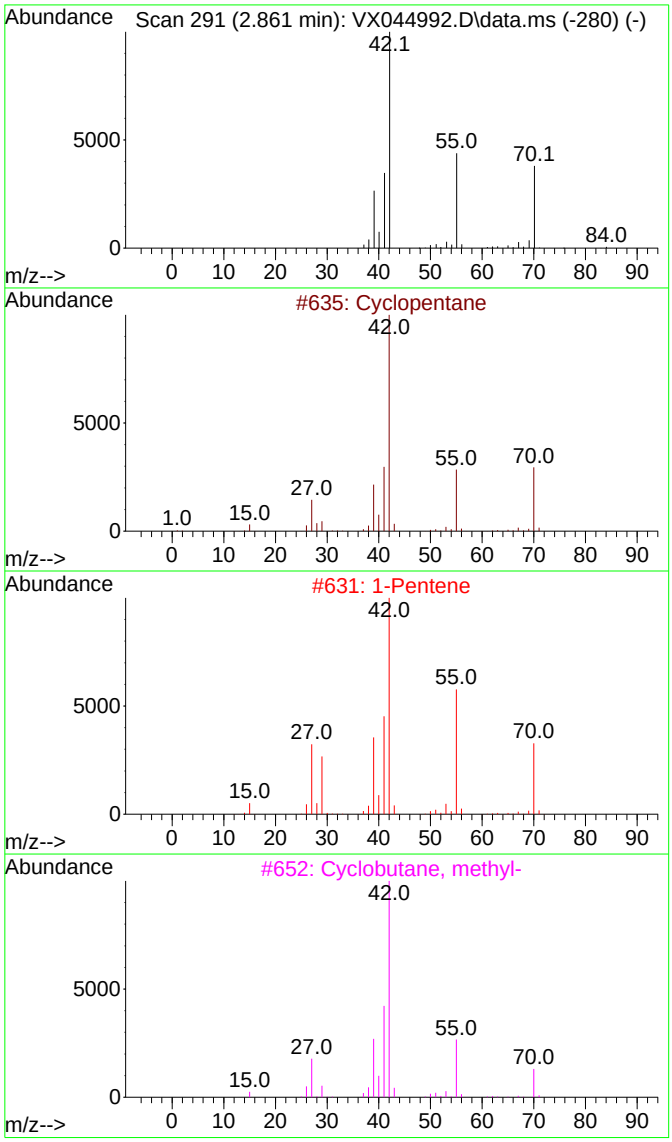
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

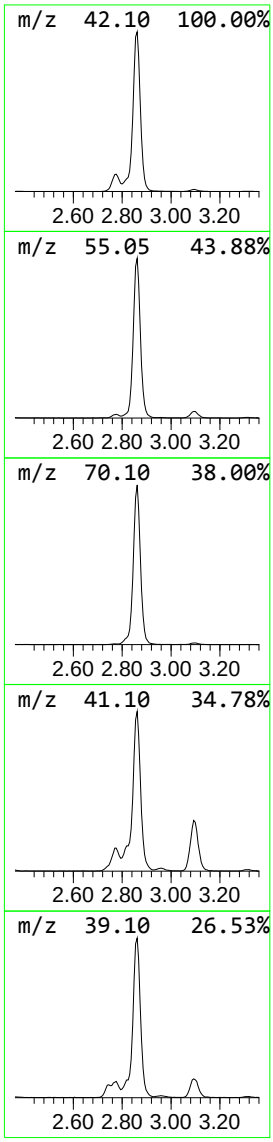
****

Peak Number 7 Cyclopentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.861	398.10 ug/l	2262900	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	1-Pentene	70	C5H10	000109-67-1	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	59
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	9
5	3-Buten-1-ol	72	C4H8O	000627-27-0	9





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Data File : VX044992.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW32

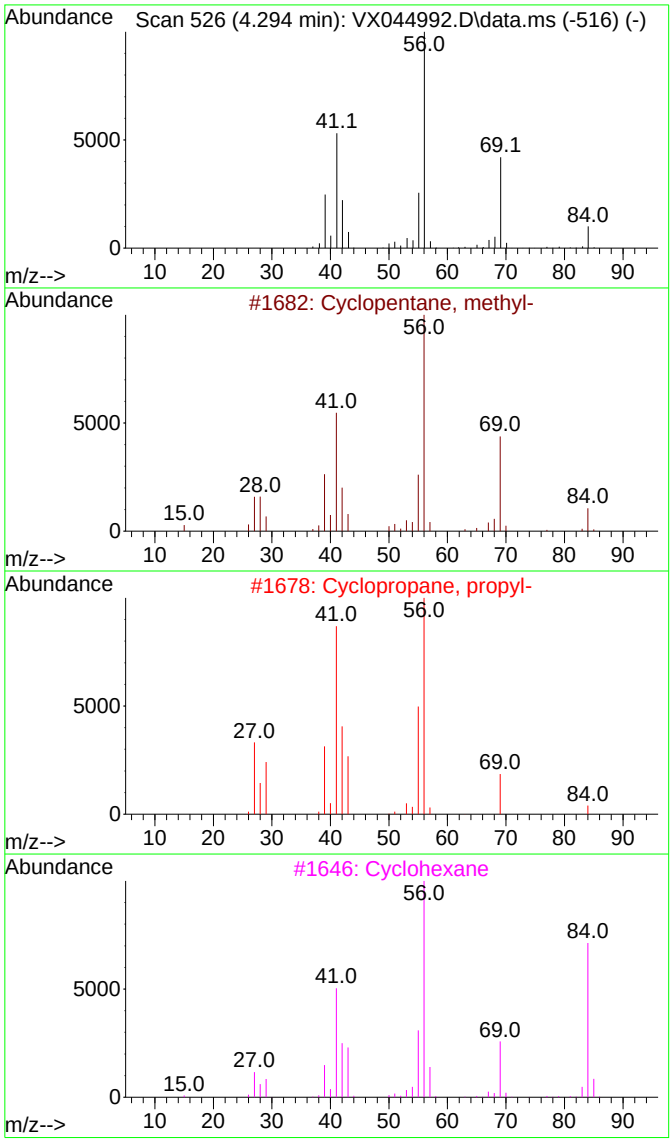
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

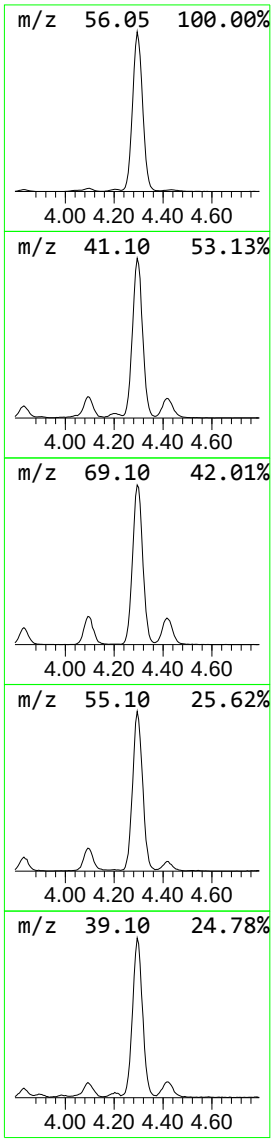
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.294	307.38 ug/l	1747270	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	78
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW32

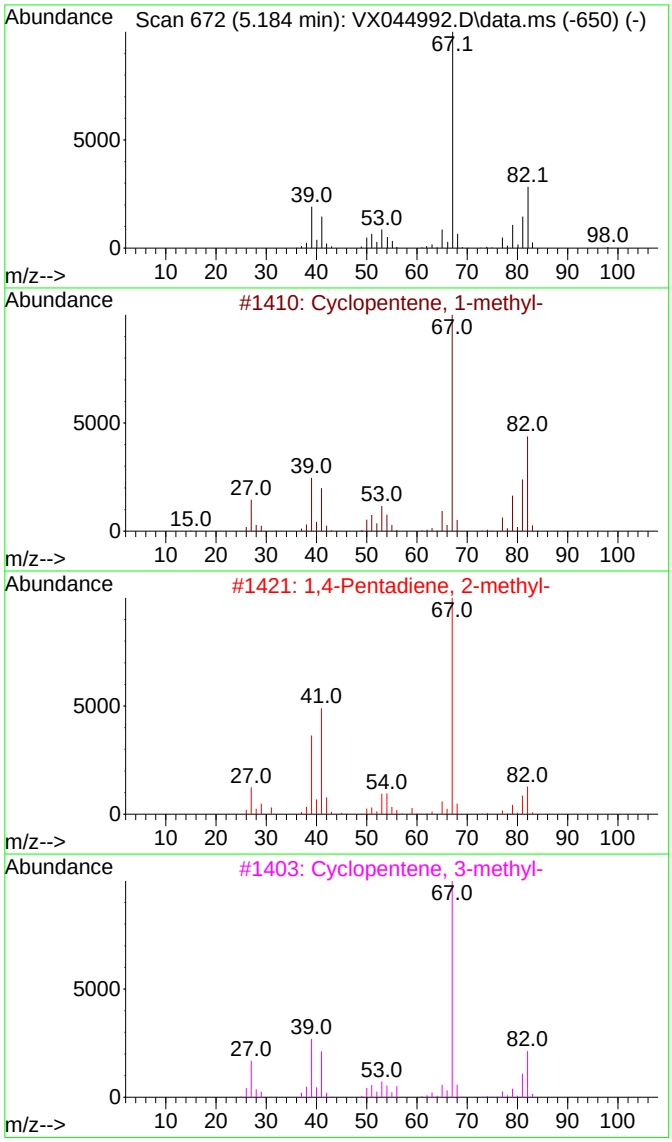
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

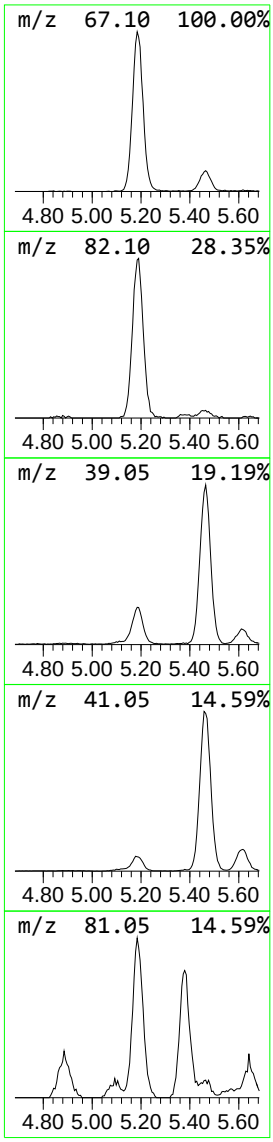
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopentene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.184	62.57 ug/l	355639	Pentafluorobenzene	5.544

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	93
2	1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	90
3	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	86
4	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	83
5	Cyclopentane, methylene-	82	C6H10	001528-30-9	83





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW32

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

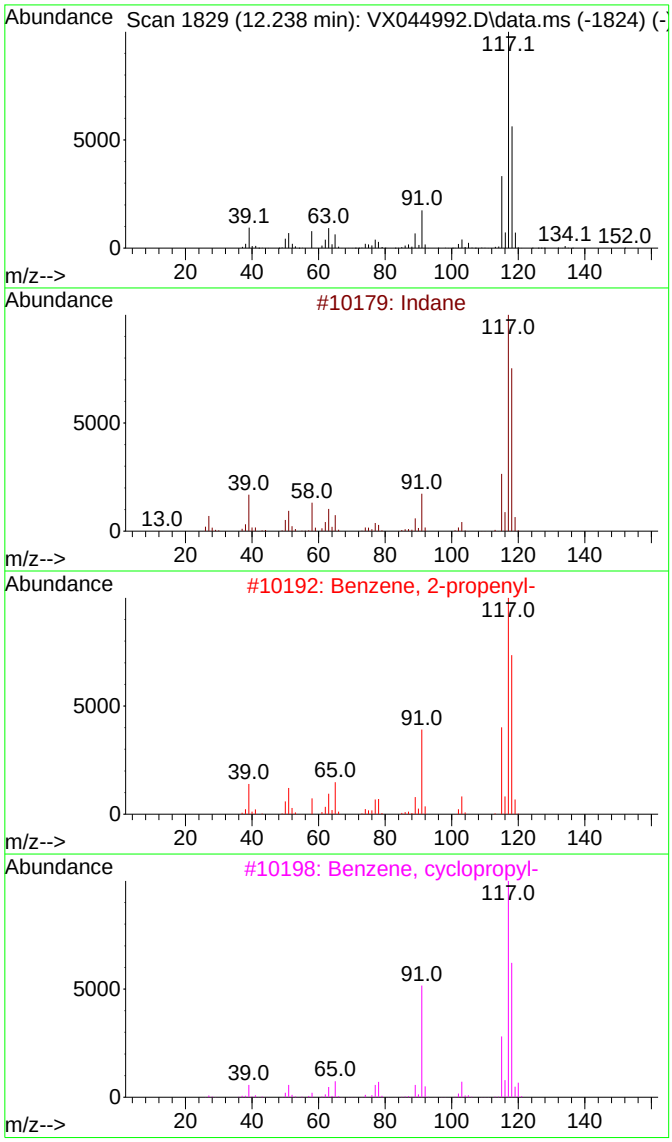
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

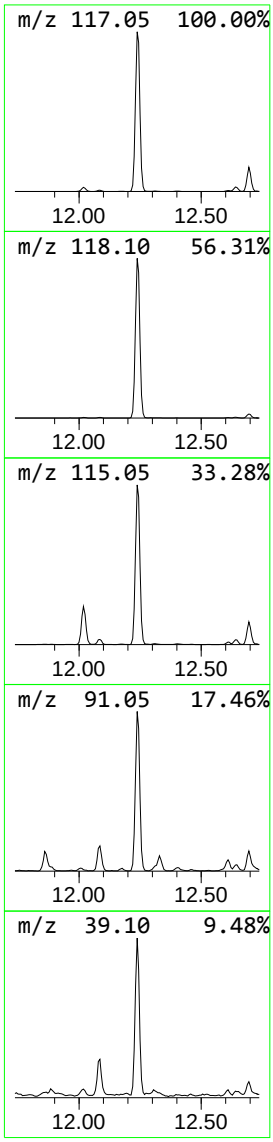
****

Peak Number 10 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.238	187.44 ug/l	1975100	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	64
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60





Tentatively Identified Compound (LSC) summary

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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
Isobutane	1.264	154.6	ug/l	878958	1	5.544	284215	50.0
Butane	1.368	511.5	ug/l	2907700	1	5.544	284215	50.0
Butane, 2-methyl-	1.733	605.9	ug/l	3444070	1	5.544	284215	50.0
Pentane	1.947	72.5	ug/l	412260	1	5.544	284215	50.0
Cyclopropane, 1...	2.209	153.6	ug/l	872899	1	5.544	284215	50.0
Butane, 2,3-dim...	2.776	69.5	ug/l	394804	1	5.544	284215	50.0
Cyclopentane	2.861	398.1	ug/l	2262900	1	5.544	284215	50.0
Cyclopentane, m...	4.294	307.4	ug/l	1747270	1	5.544	284215	50.0
Cyclopentene, 1...	5.184	62.6	ug/l	355639	1	5.544	284215	50.0
Indane	12.238	187.4	ug/l	1975100	4	12.018	526852	50.0