LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	93	rBV	543744	598680	58.15%	6.125%
2	1.605	161	167	171	rVB4	7421	13322	1.29%	0.136%
3	1.794	192	198	211	rVB	154453	223064	21.66%	2.282%
4	2.398	290	297	303	rBV5	8663	20285	1.97%	0.208%
5	2.849	362	371	386	rBV	185097	410684	39.89%	4.201%
6	3.178	417	425	434	rBV	22923	52324	5.08%	0.535%
7	4.312	596	611	626	rBV2	75282	236927	23.01%	2.424%
8	4.611	641	660	673	rBV3	38279	129402	12.57%	1.324%
9	5.513	796	808	818	rBV2	85129	242341	23.54%	2.479%
10	5.678	825	835	840	rBV2	135323	404660	39.30%	4.140%
11	5.733	840	844	858	rVB2	130926	368517	35.79%	3.770%
12	5.952	871	880	891	rVB5	9134	28936	2.81%	0.296%
13	6.080	891	901	911	rBV	97178	254924	24.76%	2.608%
14	6.269	922	932	935	rBV4	10666	26637	2.59%	0.273%
15	6.354	935	946	958	rVB	337263	1029616	100.00%	10.533%
16	6.873	1020	1031	1047	rBV	218596	524756	50.97%	5.368%
17	7.226	1081	1089	1100	rVB3	14953	33557	3.26%	0.343%
18	7.458	1119	1127	1135	rBV4	13296	34795	3.38%	0.356%
19	7.586	1140	1148	1153	rBV	40642	86527	8.40%	0.885%
20	7.641	1153	1157	1161	rVV2	29532	60868	5.91%	0.623%
21	7.689	1161	1165	1173	rVB	29894	61535	5.98%	0.630%
22	7.854	1186	1192	1200	rVB2	8186	17455	1.70%	0.179%
23	8.061	1216	1226	1238	rBV	260005	529434	51.42%	5.416%
24	8.183	1238	1246	1254	rVV	330617	672425	65.31%	6.879%
25	8.263	1254	1259	1276	rVB	22680	52686	5.12%	0.539%
26	8.458	1287	1291	1296	rVB2	7726	13232	1.29%	0.135%
27	8.519	1296	1301	1308	rVB3	12033	21681	2.11%	0.222%
28	8.689	1321	1329	1331	rBV	85312	155333	15.09%	1.589%
29	8.726	1331	1335	1350	rVV	442047	727096	70.62%	7.438%
30	8.848	1350	1355	1359	rVB3	7841	13331	1.29%	0.136%
31	9.049	1382	1388	1393	rBV3	11288	19215	1.87%	0.197%
32	9.268	1419	1424	1429	rVB3	12415	19687	1.91%	0.201%
33	10.122	1559	1564	1583	rVB2	485888	803208	78.01%	8.217%
34	10.445	1610	1617	1622	rVB4	6696	10349	1.01%	0.106%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Title : SW846 8260

35	10.658	1641	1652	1653	rBV6	6077	13532	1.31%	0.138%
36	10.841	1680	1682	1691	rVB5	6292	11115	1.08%	0.114%
37	11.079	1715	1721	1726	rVV	17668	27296	2.65%	0.279%
38	11.146	1726	1732	1737	rVV	429780	535915	52.05%	5.483%
39	11.183	1737	1738	1744	rVB3	11116	11548	1.12%	0.118%
40	11.683	1810	1820	1826	rBV7	7706	16306	1.58%	0.167%
41	11.780	1826	1836	1839	rBV2	12721	18265	1.77%	0.187%
42	11.933	1853	1861	1862	rBV2	14143	19911	1.93%	0.204%
43	11.957	1862	1865	1871	rVB	14472	18892	1.83%	0.193%
44	12.085	1881	1886	1898	rVB	583109	751293	72.97%	7.686%
45	12.244	1907	1912	1916	rVV	36996	44806	4.35%	0.458%
46	12.311	1918	1923	1928	rVB	37705	47684	4.63%	0.488%
47	12.378	1928	1934	1944	rVB6	12236	23758	2.31%	0.243%
48	12.469	1944	1949	1954	rBV2	9546	13268	1.29%	0.136%
49	12.676	1978	1983	1986	rBV	25336	31125	3.02%	0.318%
50	12.713	1986	1989	1993	rVV2	26769	35818	3.48%	0.366%
51	12.768	1993	1998	2004	rVV2	76746	117914	11.45%	1.206%
52	12.902	2013	2020	2026	rBV	24750	38962	3.78%	0.399%
53	12.969	2026	2031	2032	rBV2	7880	10706	1.04%	0.110%
54	12.987	2032	2034	2039	rVB3	10220	12426	1.21%	0.127%
55	13.097	2047	2052	2056	rBV3	7808	10668	1.04%	0.109%
56	13.359	2090	2095	2100	rVB3	21984	30080	2.92%	0.308%
57	13.487	2107	2116	2121	rBV6	9130	12824	1.25%	0.131%
58	13.652	2139	2143	2146	rBV	7792	10368	1.01%	0.106%
59	13.707	2146	2152	2154	rVV4	7083	13003	1.26%	0.133%

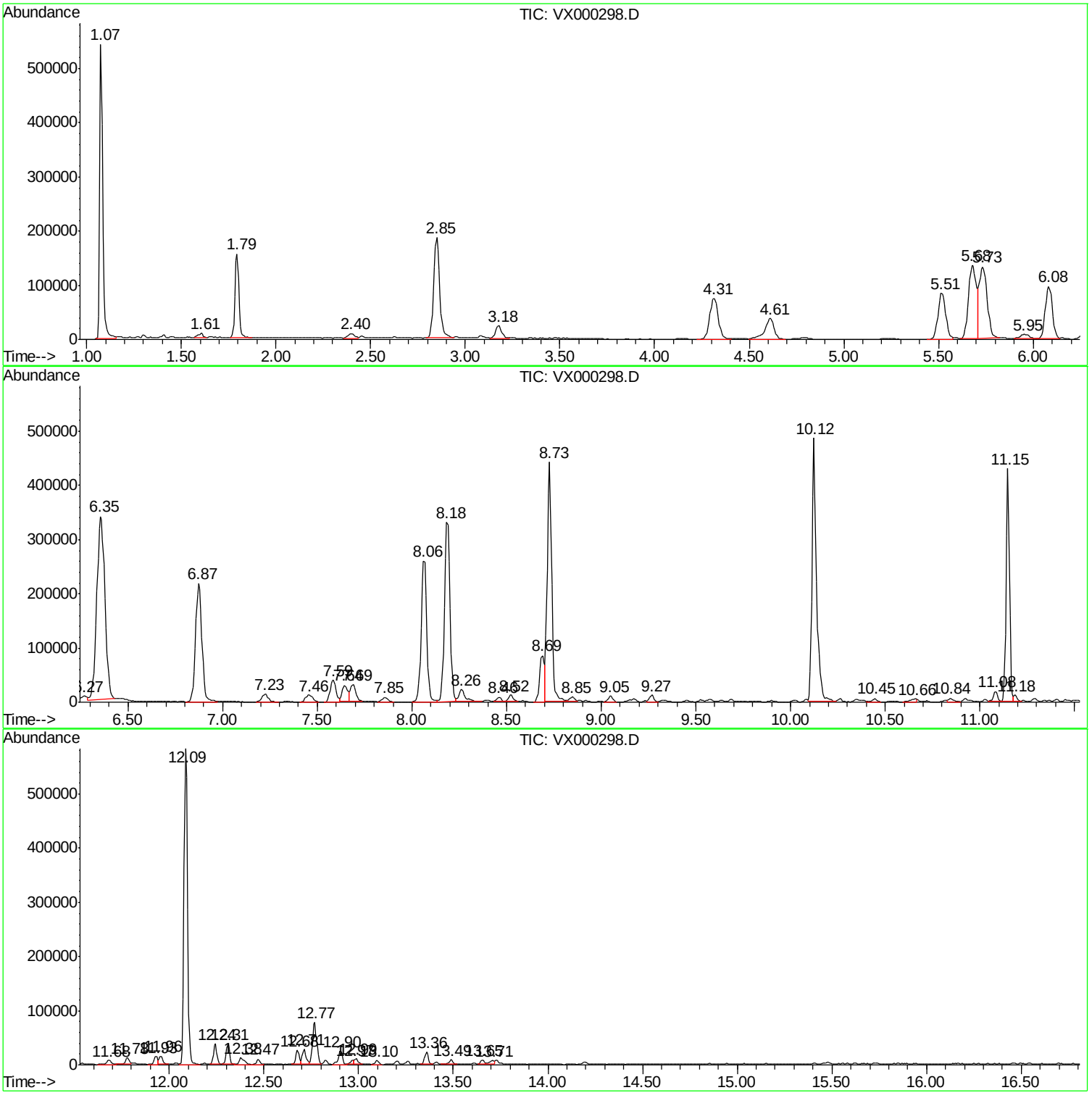
Sum of corrected areas: 9774972

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

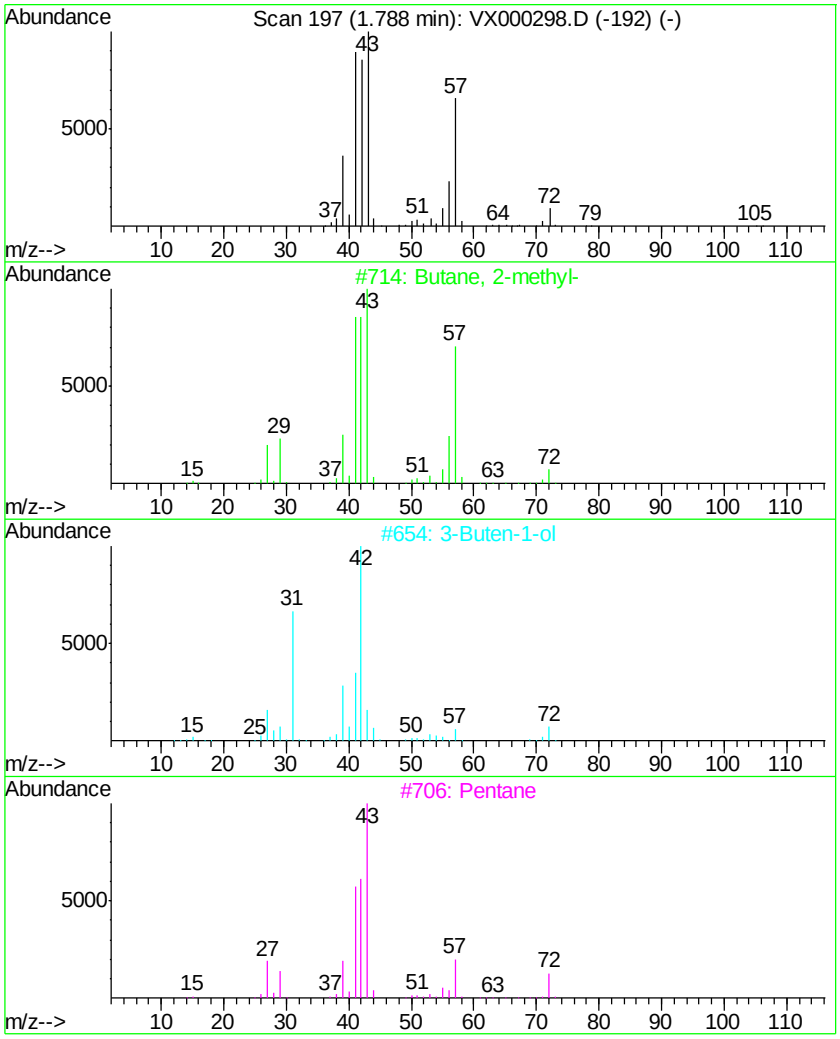
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

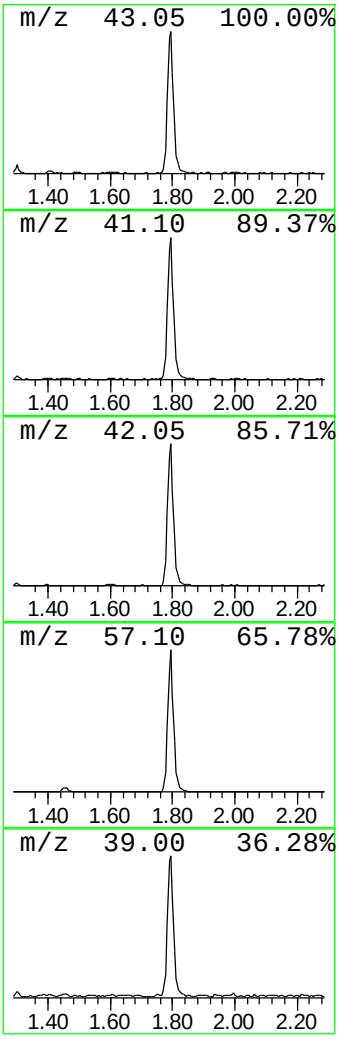
****

Peak Number 2 Butane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	27.56 ug/l	223064	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	3-Buten-1-ol	72	C4H8O	000627-27-0	37
3	Pentane	72	C5H12	000109-66-0	28
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

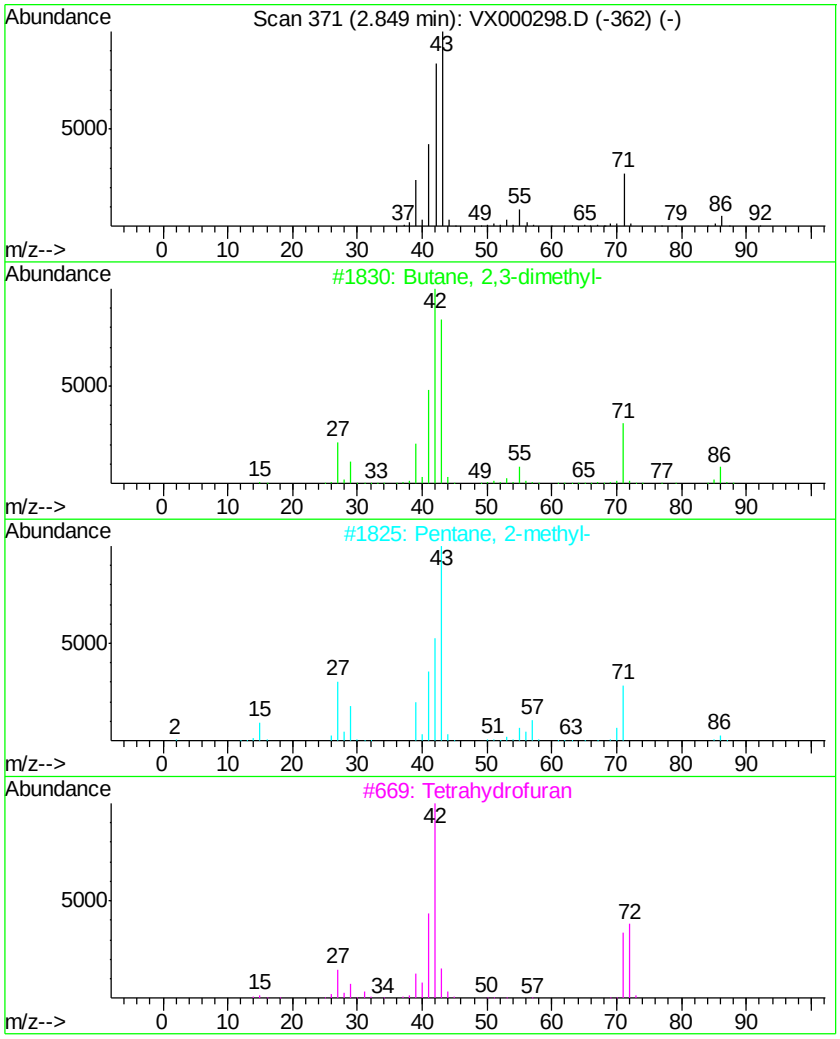
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

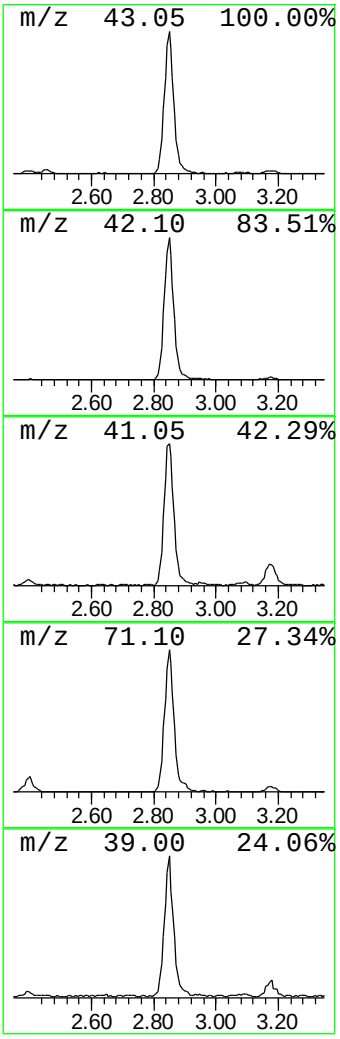
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	50.74 ug/l	410684	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	36
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

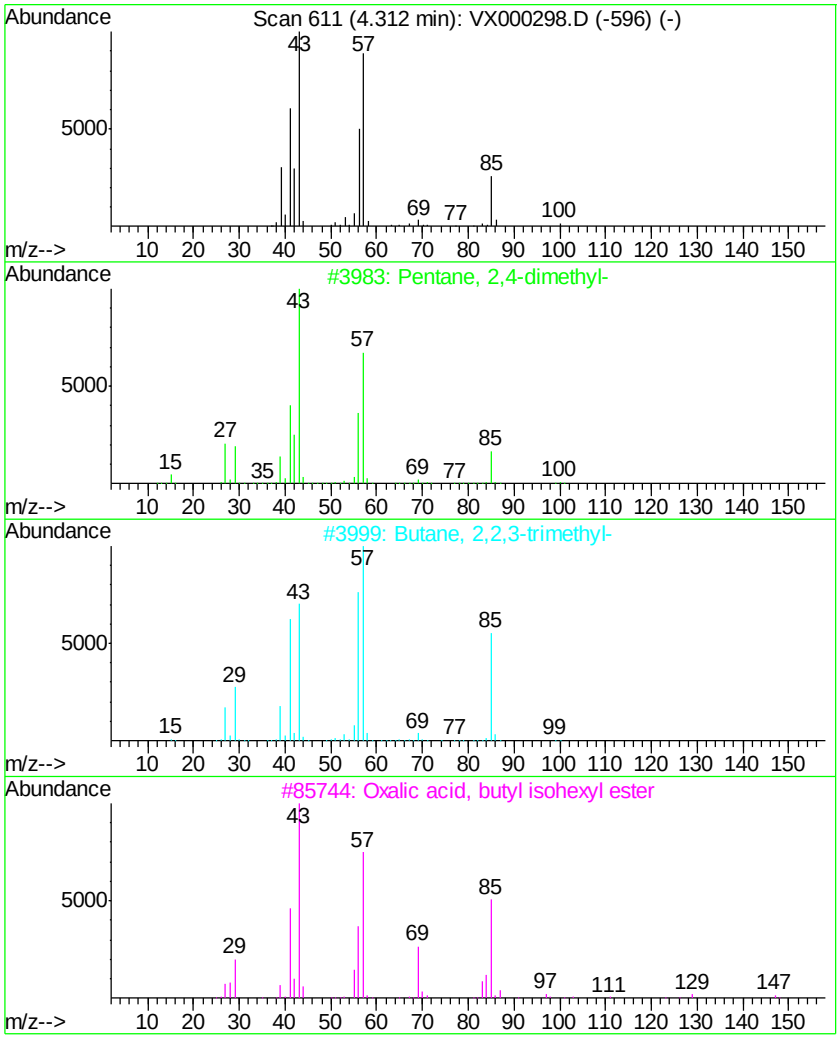
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

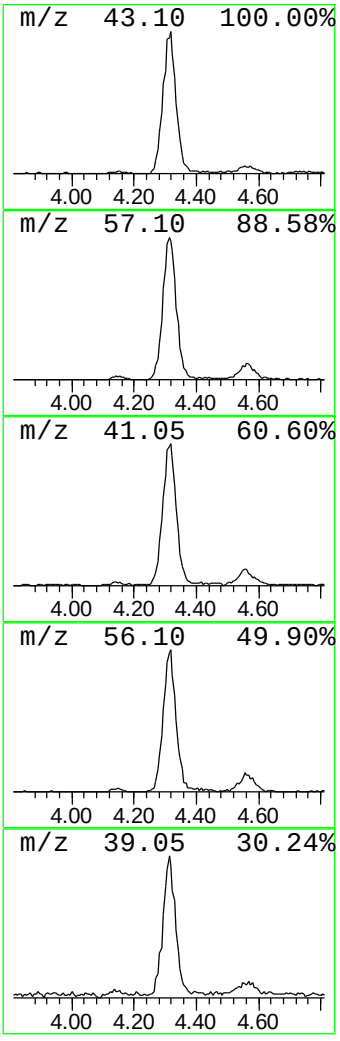
****

Peak Number 4 Pentane, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.31	29.27 ug/l	236927	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	72
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
3	Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59
4	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53
5	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	40





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

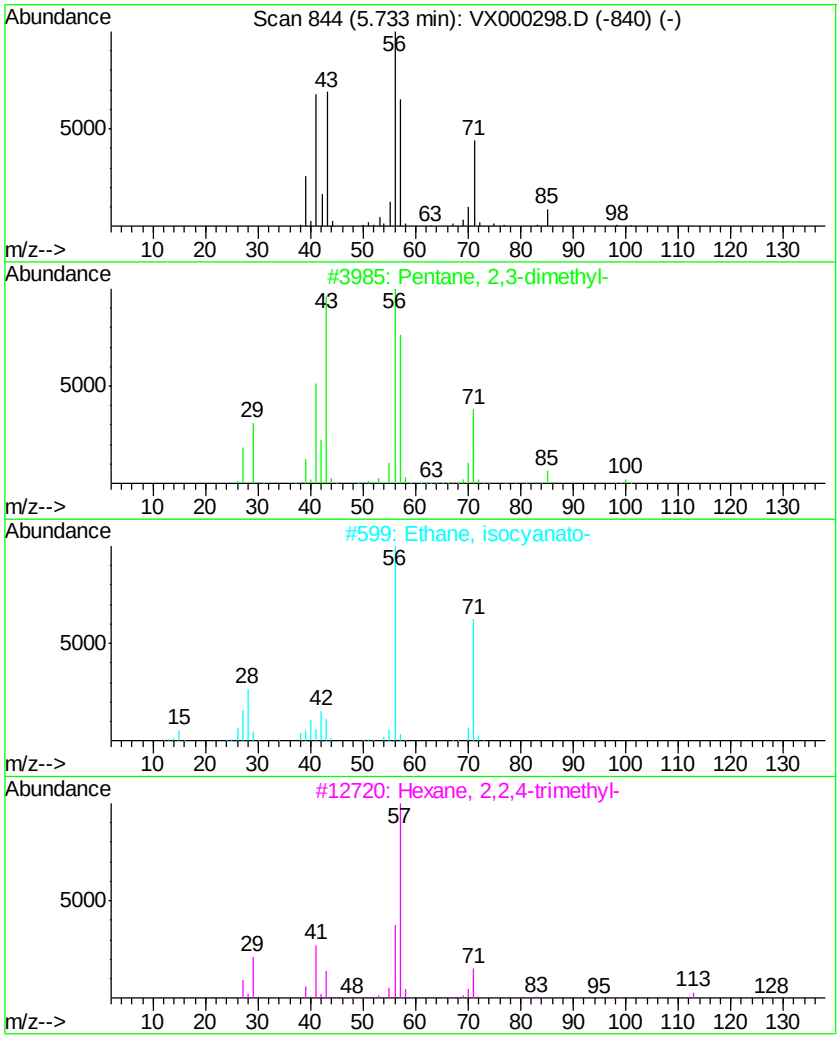
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

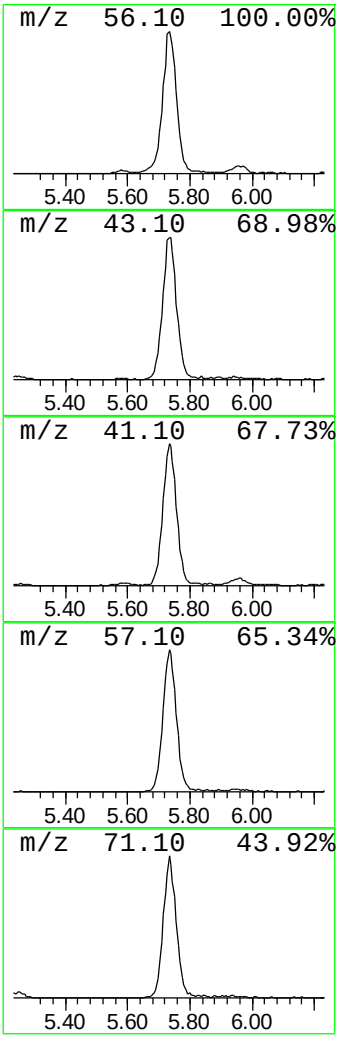
****

Peak Number 5 Pentane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.73	45.53 ug/l	368517	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	74
2	Ethane, isocyanato-	71	C3H5NO	000109-90-0	64
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53
4	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	50
5	5,5-Dimethyl-1,3-dioxan-2-one	130	C6H10O3	003592-12-9	50





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

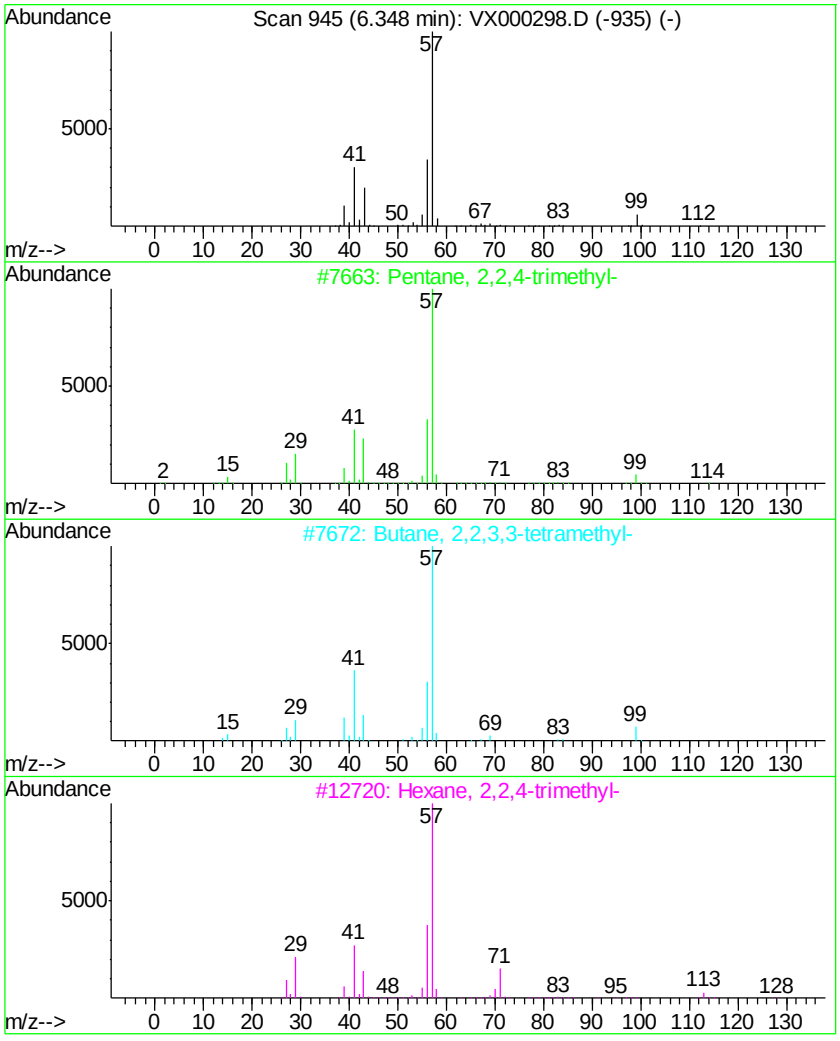
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

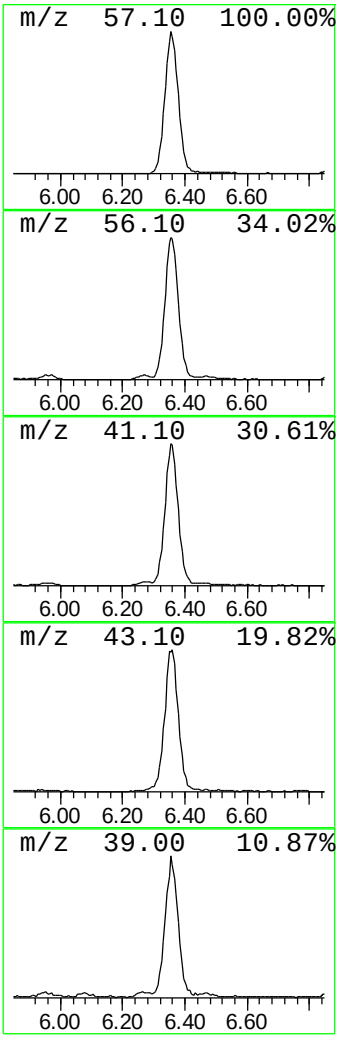
****

Peak Number 6 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	98.10 ug/l	1029620	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
4	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

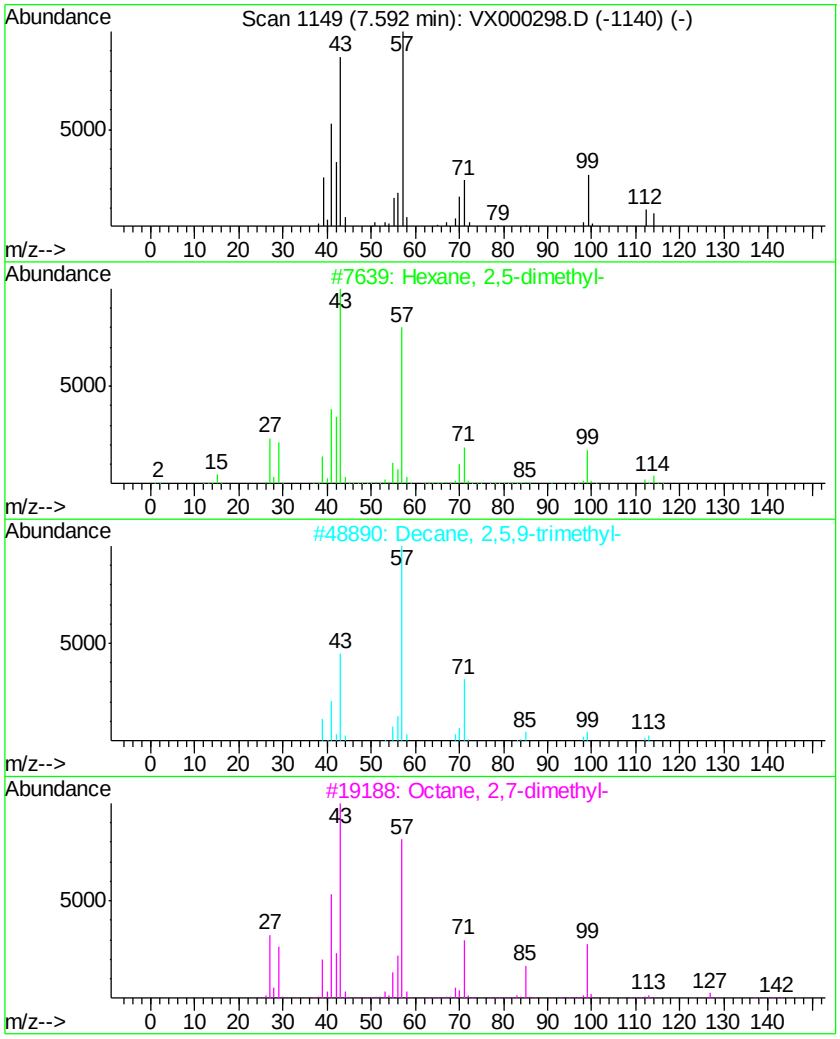
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

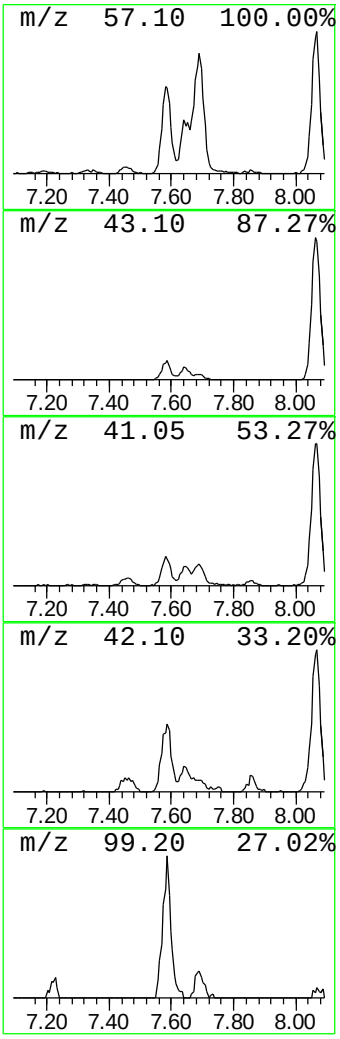
****

Peak Number 7 Hexane, 2,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	8.24 ug/l	86527	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	72
2	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	47
3	Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	47
4	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	47
5	Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	43





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

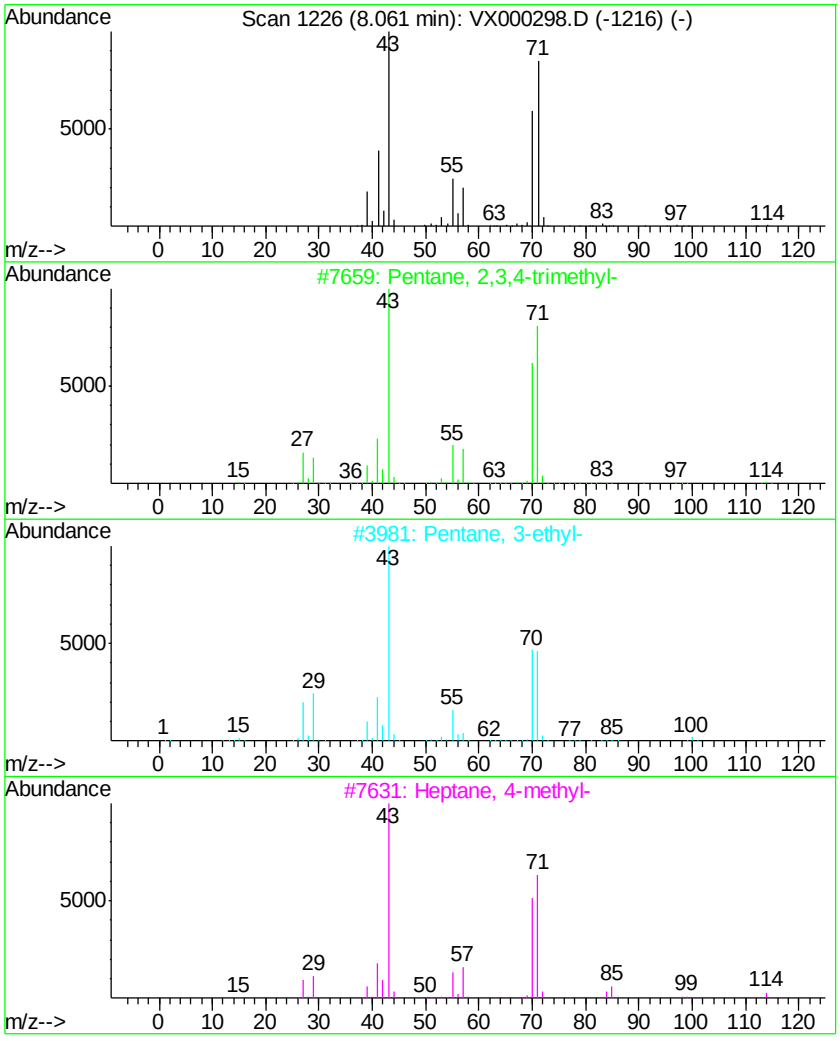
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

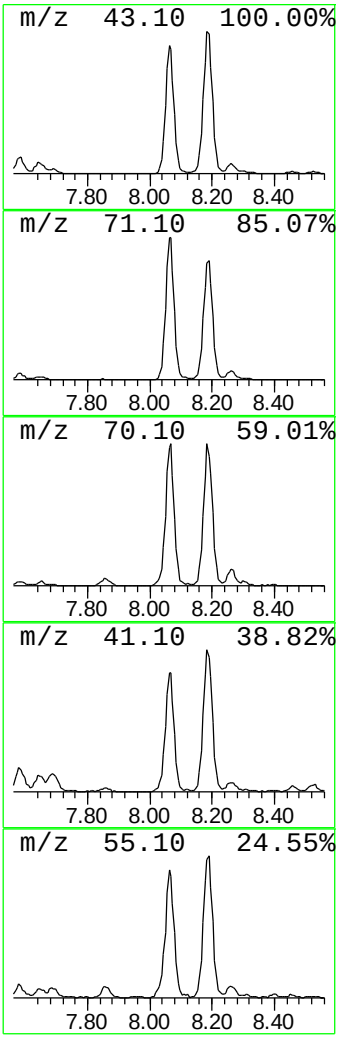
****

Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	50.45 ug/l	529434	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2	Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	78
5	Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

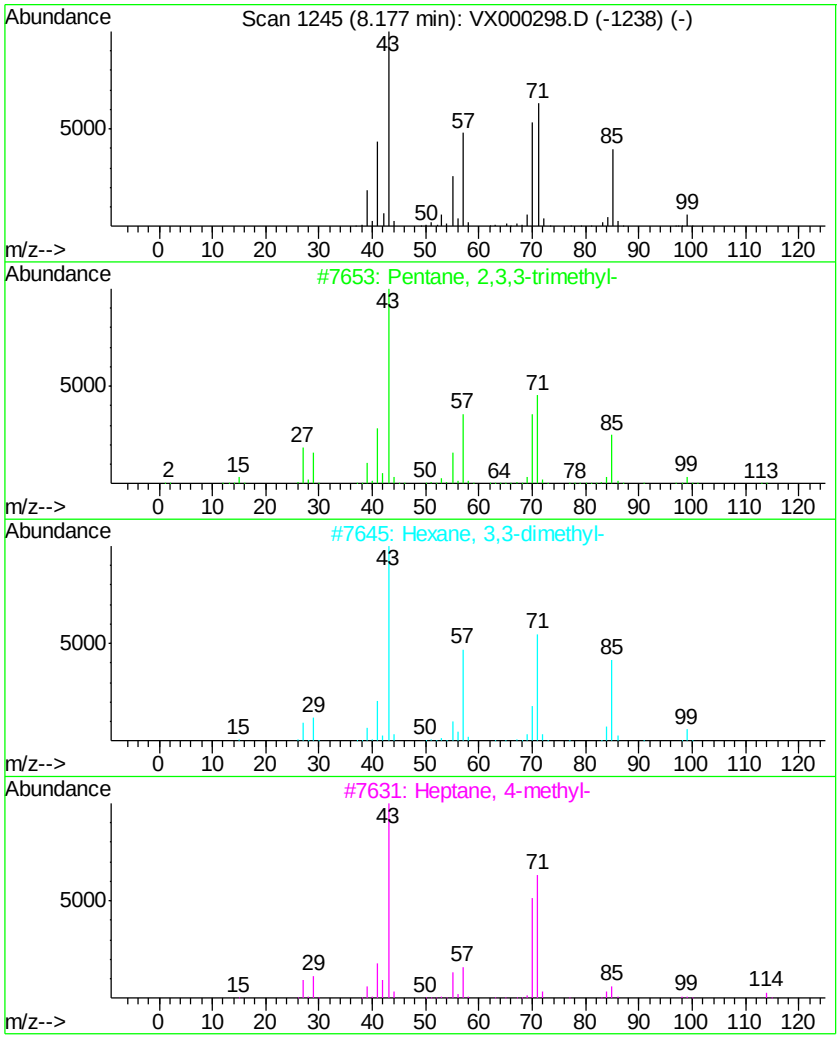
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

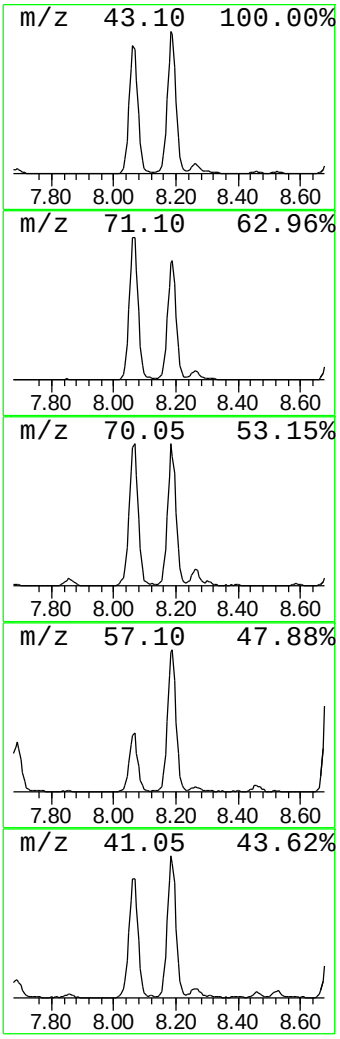
****

Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	64.07 ug/l	672425	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
4	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50
5	Pentane, 3-ethyl-	100	C7H16	000617-78-7	47





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

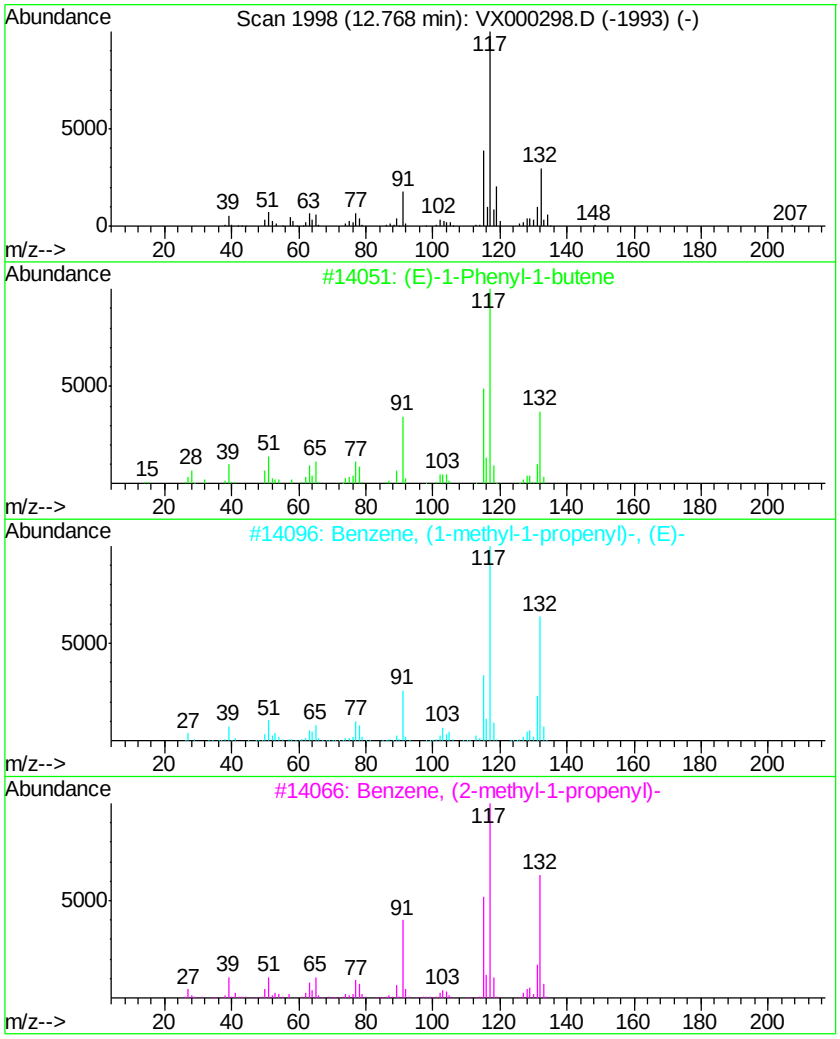
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

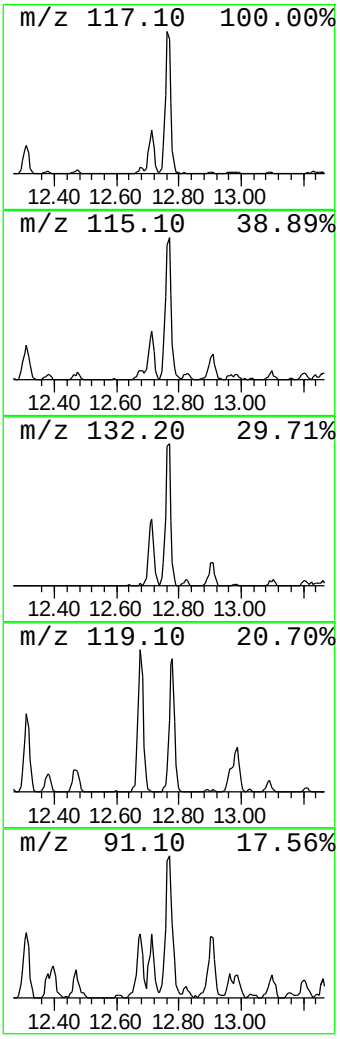
****

Peak Number 10 (E)-1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.77	7.85 ug/l	117914	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	87
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
4	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	76
5	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	74





Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX031318\
Data File : VX000298.D
Acq On : 13 Mar 2018 14:10
Operator : JC/MD
Sample : J1849-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : ST008MW038-180307

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X030718W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	1.79	27.6	ug/l	223064	1	5.68	404660	50.0
Butane, 2,3-dimet...	2.85	50.7	ug/l	410684	1	5.68	404660	50.0
Pentane, 2,4-dime...	4.31	29.3	ug/l	236927	1	5.68	404660	50.0
Pentane, 2,3-dime...	5.73	45.5	ug/l	368517	1	5.68	404660	50.0
Pentane, 2,2,4-tr...	6.35	98.1	ug/l	1029620	2	6.87	524756	50.0
Hexane, 2,5-dimet...	7.59	8.2	ug/l	86527	2	6.87	524756	50.0
Pentane, 2,3,4-tr...	8.06	50.5	ug/l	529434	2	6.87	524756	50.0
Pentane, 2,3,3-tr...	8.18	64.1	ug/l	672425	2	6.87	524756	50.0
(E)-1-Phenyl-1-bu...	12.77	7.8	ug/l	117914	4	12.09	751293	50.0