LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

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\82X091118W.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	1.788	100	104	111	rVB	16767	23557	1.72%	0.208%
2	2.391	198	203	208	rBV	15812	29013	2.12%	0.256%
3	2.611	234	239	248	rVB	15075	27235	1.99%	0.240%
4	2.843	270	277	283	rBV	22186	49833	3.65%	0.440%
5	2.928	288	291	304	rVB3	6257	14457	1.06%	0.128%
6	3.166	322	330	343	rVB	56739	131567	9.63%	1.161%
7	4.141	477	490	502	rBV2	8198	25729	1.88%	0.227%
8	4.306	504	517	523	rVV3	7872	24446	1.79%	0.216%
9	4.397	523	532	545	rVV3	43455	130659	9.57%	1.153%
10	4.556	547	558	576	rVB4	4856	19433	1.42%	0.172%
11	5.232	655	669	683	rBV2	14620	50941	3.73%	0.450%
12	5.507	701	714	721	rBV	174928	511812	37.48%	4.518%
13	5.574	721	725	731	rVV2	40440	105185	7.70%	0.929%
14	5.665	731	740	765	rVB	259342	803391	58.83%	7.092%
15	5.946	773	786	796	rBV3	18167	58503	4.28%	0.516%
16	6.068	796	806	826	rVV2	193449	491185	35.97%	4.336%
17	6.263	828	838	847	rVV4	19781	76364	5.59%	0.674%
18	6.354	847	853	861	rVV3	19030	52957	3.88%	0.467%
19	6.452	861	869	880	rVB3	31429	89695	6.57%	0.792%
20	6.860	926	936	955	rBV	356538	832258	60.94%	7.347%
21	7.458	1021	1034	1044	rBV3	112554	271331	19.87%	2.395%
22	7.634	1058	1063	1074	rVV2	5935	13801	1.01%	0.122%
23	7.848	1090	1098	1107	rVB3	17317	37081	2.72%	0.327%
24	8.031	1115	1128	1138	rVB3	18071	43959	3.22%	0.388%
25	8.390	1179	1187	1193	rBV2	18223	33709	2.47%	0.298%
26	8.665	1224	1232	1235	rBV2	54971	95541	7.00%	0.843%
27	8.713	1235	1240	1255	rVV	842665	1365700	100.00%	12.056%
28	8.841	1255	1261	1266	rVV	35937	61631	4.51%	0.544%
29	8.909	1266	1272	1279	rVB	16217	31455	2.30%	0.278%
30	9.043	1288	1294	1300	rBV	80954	132348	9.69%	1.168%
31	9.165	1306	1314	1320	rBV2	36860	61257	4.49%	0.541%
32	9.445	1353	1360	1369	rVB5	9235	17638	1.29%	0.156%
33	9.567	1374	1380	1385	rBV2	26335	51146	3.75%	0.451%
34	9.622	1385	1389	1394	rVB	38299	53010	3.88%	0.468%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

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\82X091118W.M
Title : SW846 8260

35	9.677	1394	1398	1403	rBV	71753	104474	7.65%	0.922%
36	9.890	1426	1433	1438	rBV4	16329	32253	2.36%	0.285%
37	10.116	1464	1470	1477	rBV	710855	956180	70.01%	8.441%
38	10.189	1477	1482	1486	rVB	21628	33790	2.47%	0.298%
39	10.238	1486	1490	1497	rVB2	12911	22178	1.62%	0.196%
40	10.335	1501	1506	1508	rBV2	28159	41541	3.04%	0.367%
41	10.512	1531	1535	1542	rVB	15339	21830	1.60%	0.193%
42	10.646	1545	1557	1565	rBV4	21609	62746	4.59%	0.554%
43	10.835	1585	1588	1593	rVB	21013	28004	2.05%	0.247%
44	10.914	1596	1601	1605	rBV3	12864	23305	1.71%	0.206%
45	11.018	1613	1618	1622	rBV	24436	30990	2.27%	0.274%
46	11.140	1632	1638	1643	rBV	708394	885237	64.82%	7.814%
47	11.183	1643	1645	1649	rVB4	12631	15225	1.11%	0.134%
48	11.280	1657	1661	1669	rVB2	27315	41731	3.06%	0.368%
49	11.359	1670	1674	1678	rBV	22882	30028	2.20%	0.265%
50	11.451	1684	1689	1692	rBV3	9451	17156	1.26%	0.151%
51	11.670	1717	1725	1732	rVV4	16249	30839	2.26%	0.272%
52	11.914	1758	1765	1767	rBV3	9655	18633	1.36%	0.164%
53	11.945	1767	1770	1775	rVB	16169	23779	1.74%	0.210%
54	12.079	1787	1792	1798	rBV	884771	1077449	78.89%	9.511%
55	12.146	1798	1803	1807	rVB	64953	83265	6.10%	0.735%
56	12.231	1812	1817	1821	rVV	21283	29917	2.19%	0.264%
57	12.304	1825	1829	1834	rVV	51258	62863	4.60%	0.555%
58	12.371	1834	1840	1848	rVB3	28284	54578	4.00%	0.482%
59	12.463	1848	1855	1859	rBV	28967	38933	2.85%	0.344%
60	12.670	1885	1889	1892	rBV	51051	58259	4.27%	0.514%
61	12.707	1892	1895	1900	rVB2	21538	31926	2.34%	0.282%
62	12.768	1900	1905	1910	rVB3	59919	104927	7.68%	0.926%
63	12.871	1918	1922	1924	rBV	20995	29626	2.17%	0.262%
64	12.902	1924	1927	1932	rVB2	60060	79956	5.85%	0.706%
65	12.981	1932	1940	1944	rBV2	64979	99190	7.26%	0.876%
66	13.042	1944	1950	1953	rBV5	13447	20889	1.53%	0.184%
67	13.085	1953	1957	1962	rVB3	20932	35396	2.59%	0.312%
68	13.152	1962	1968	1972	rBV	23528	34924	2.56%	0.308%
69	13.194	1972	1975	1978	rBV2	24706	26939	1.97%	0.238%
70	13.310	1989	1994	1996	rBV2	15323	25293	1.85%	0.223%
71	13.347	1996	2000	2006	rVB2	184271	252568	18.49%	2.230%

LSC Area Percent Report

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Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

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\82X091118W.M
Title : SW846 8260

72	13.481	2015	2022	2027	rVB3	58322	92056	6.74%	0.813%
73	13.566	2032	2036	2039	rBV4	12854	20735	1.52%	0.183%
74	13.603	2039	2042	2044	rVV	14918	18428	1.35%	0.163%
75	13.639	2044	2048	2052	rVV3	54079	85789	6.28%	0.757%
76	13.700	2052	2058	2059	rVV2	35137	62722	4.59%	0.554%
77	13.725	2059	2062	2070	rVB2	48993	83377	6.11%	0.736%
78	13.810	2070	2076	2078	rBV	23702	34644	2.54%	0.306%
79	13.853	2078	2083	2088	rVB2	30653	53707	3.93%	0.474%
80	13.914	2088	2093	2098	rVB	29092	40763	2.98%	0.360%
81	13.987	2098	2105	2109	rBV2	46648	70592	5.17%	0.623%
82	14.030	2109	2112	2116	rBV2	17535	22824	1.67%	0.201%
83	14.127	2124	2128	2132	rBV3	13646	20408	1.49%	0.180%
84	14.273	2148	2152	2158	rVB2	34824	61799	4.53%	0.546%
85	14.377	2166	2169	2173	rBV	17840	21398	1.57%	0.189%
86	14.432	2173	2178	2182	rVB2	19205	26786	1.96%	0.236%
87	14.475	2182	2185	2190	rVB	11168	15575	1.14%	0.137%
88	14.542	2191	2196	2204	rBV2	51123	75540	5.53%	0.667%
89	14.694	2219	2221	2224	rVV	15929	16705	1.22%	0.147%
90	14.731	2224	2227	2231	rVB3	12984	16152	1.18%	0.143%
91	14.840	2241	2245	2249	rBV2	36618	50218	3.68%	0.443%
92	15.249	2307	2312	2319	rVB3	10340	20542	1.50%	0.181%
93	15.554	2357	2362	2366	rBV	8932	13911	1.02%	0.123%
94	15.688	2378	2384	2388	rBV	10348	18867	1.38%	0.167%

Sum of corrected areas: 11328182

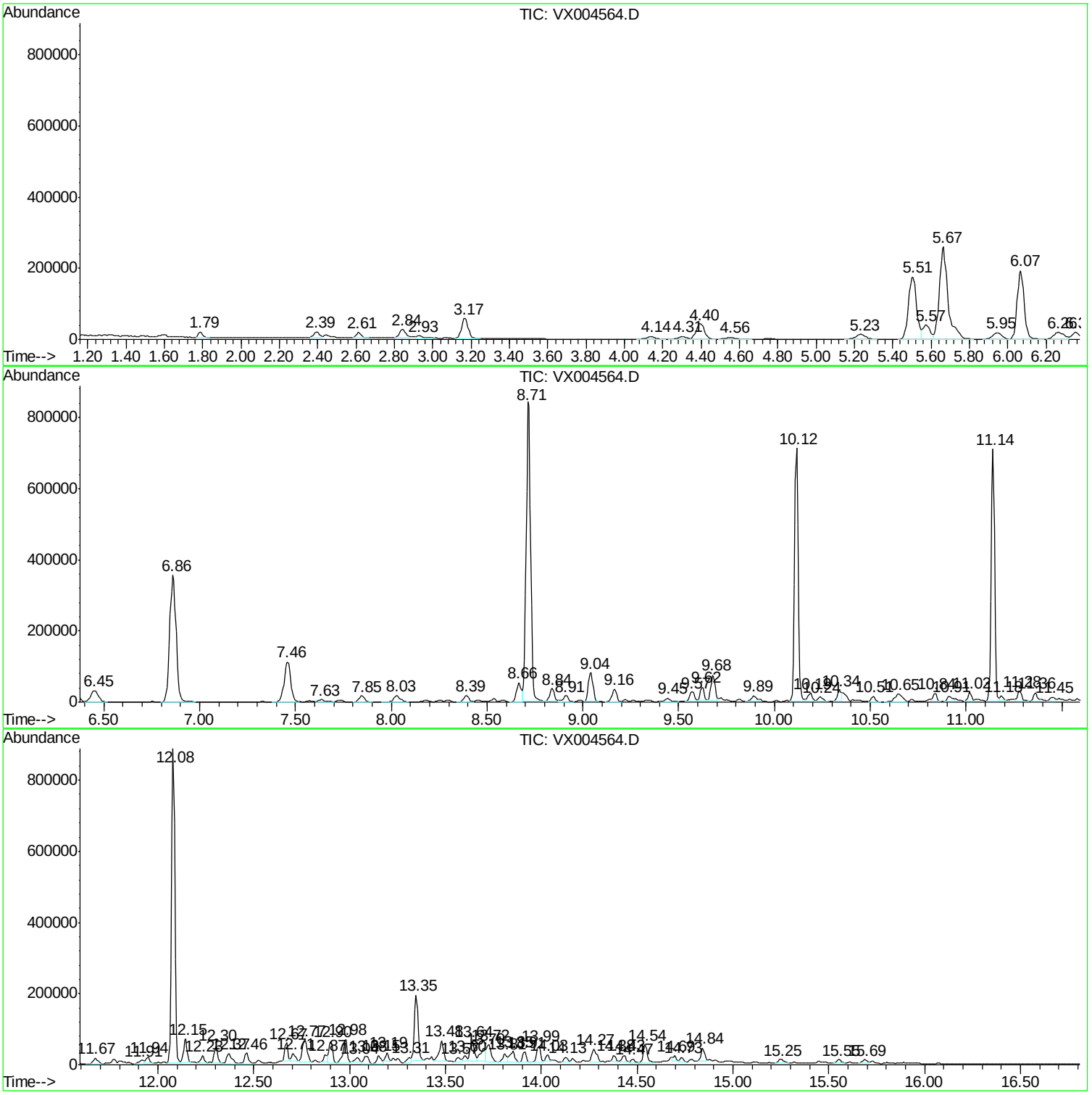
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

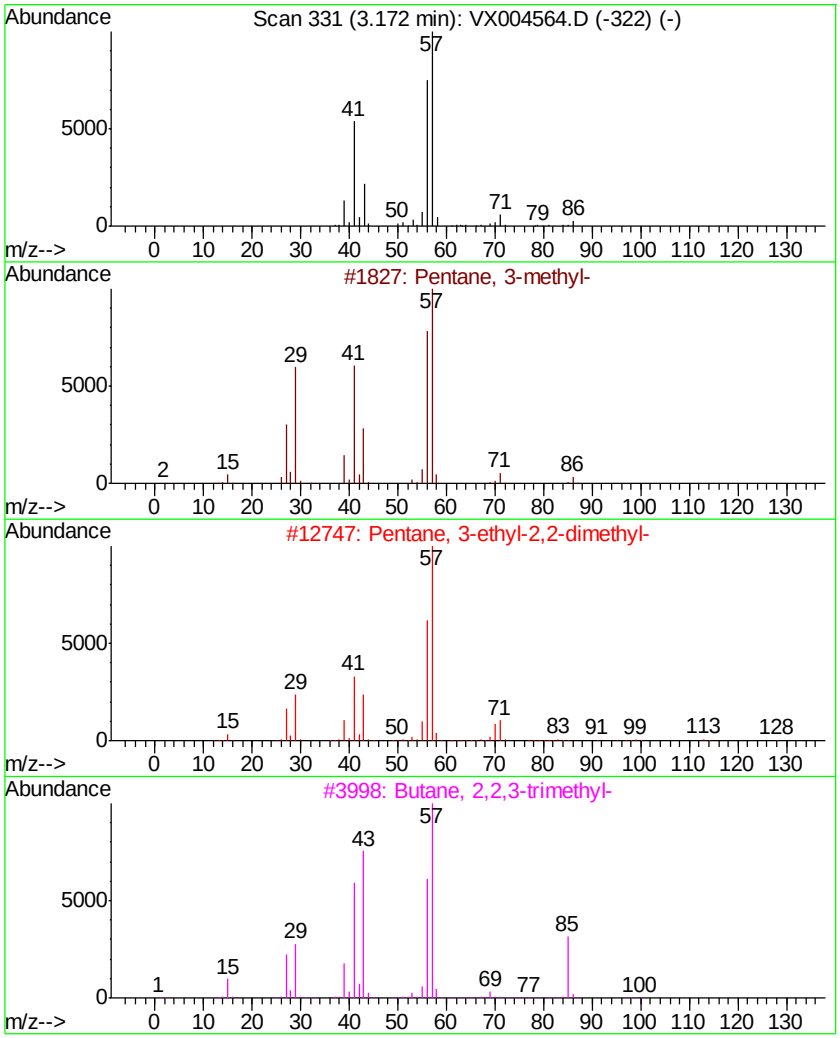
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

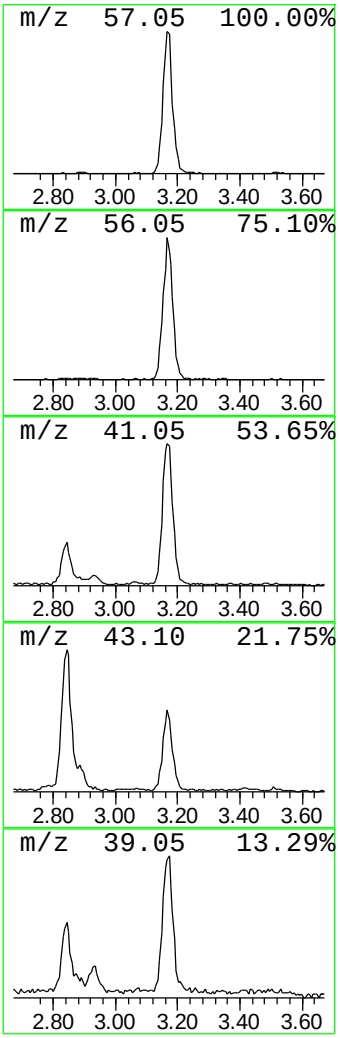
****

Peak Number 1 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	8.19 ug/l	131567	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50
3	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	50
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

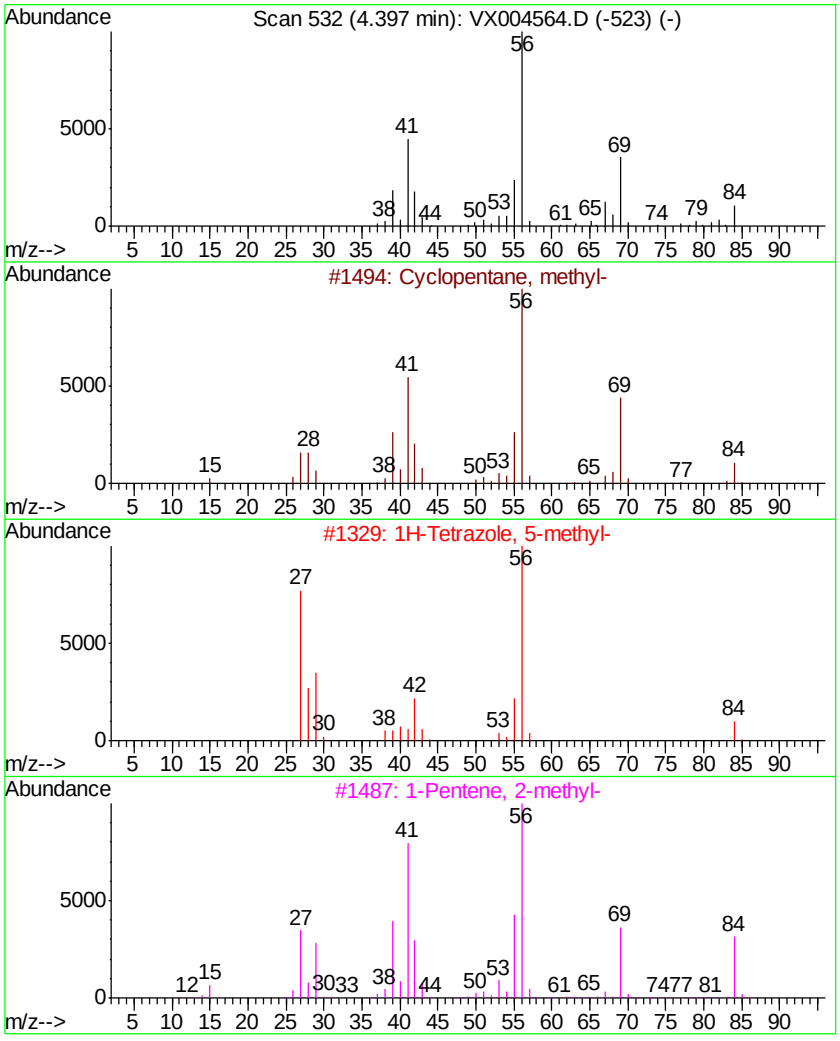
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

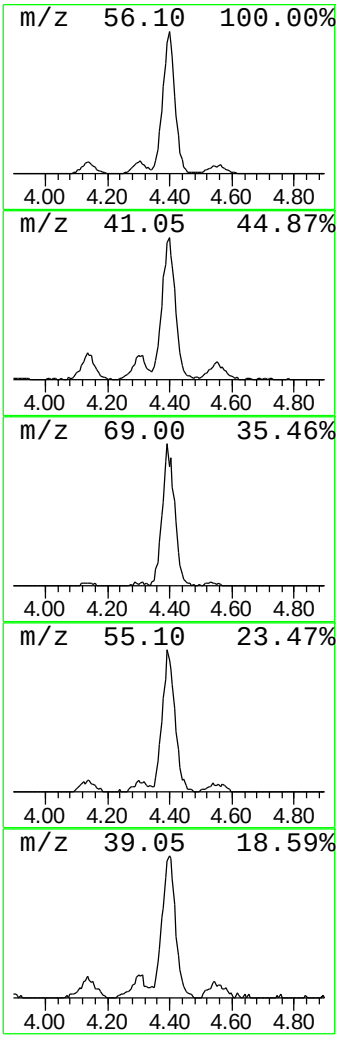
****

Peak Number 2 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	8.13 ug/l	130659	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	42
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	42
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	39





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

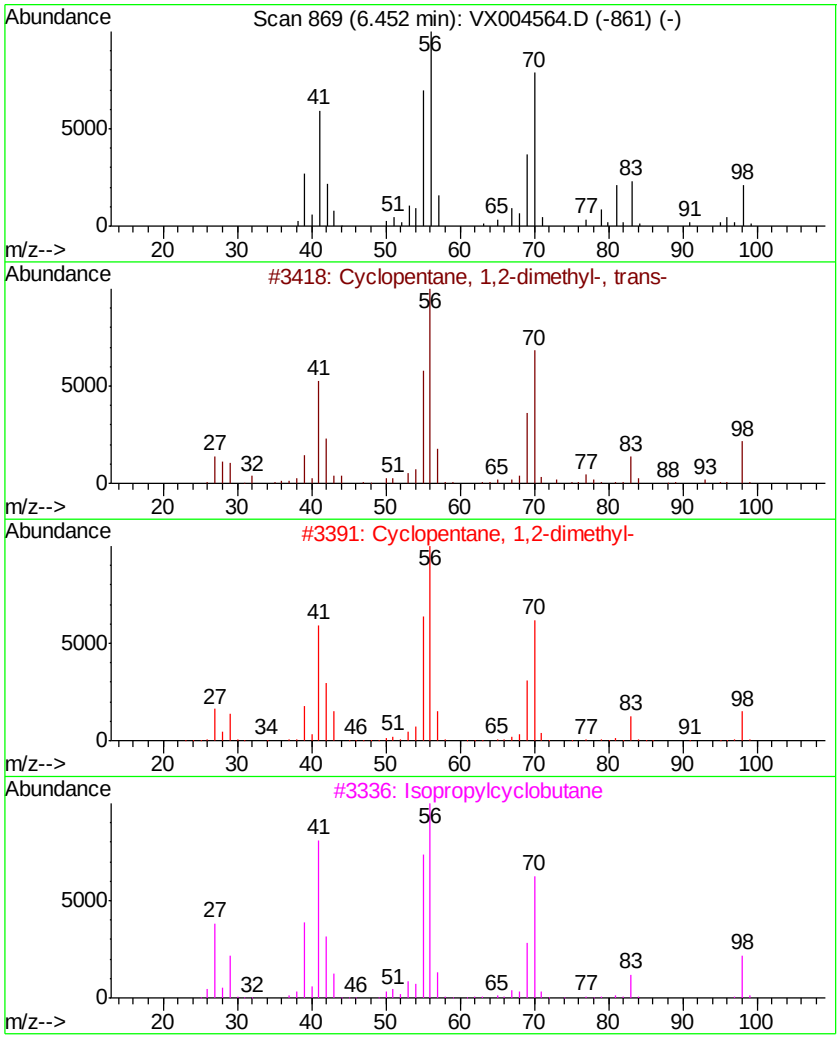
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

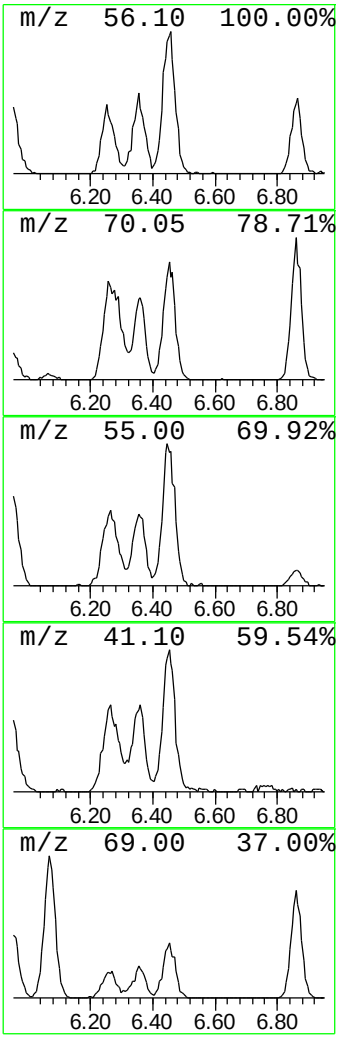
****

Peak Number 3 Cyclopentane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	5.39 ug/l	89695	1,4-Difluorobenzene	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	90
2	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	90
3	Isopropylcyclobutane	98	C7H14	000872-56-0	90
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	86
5	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	86





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

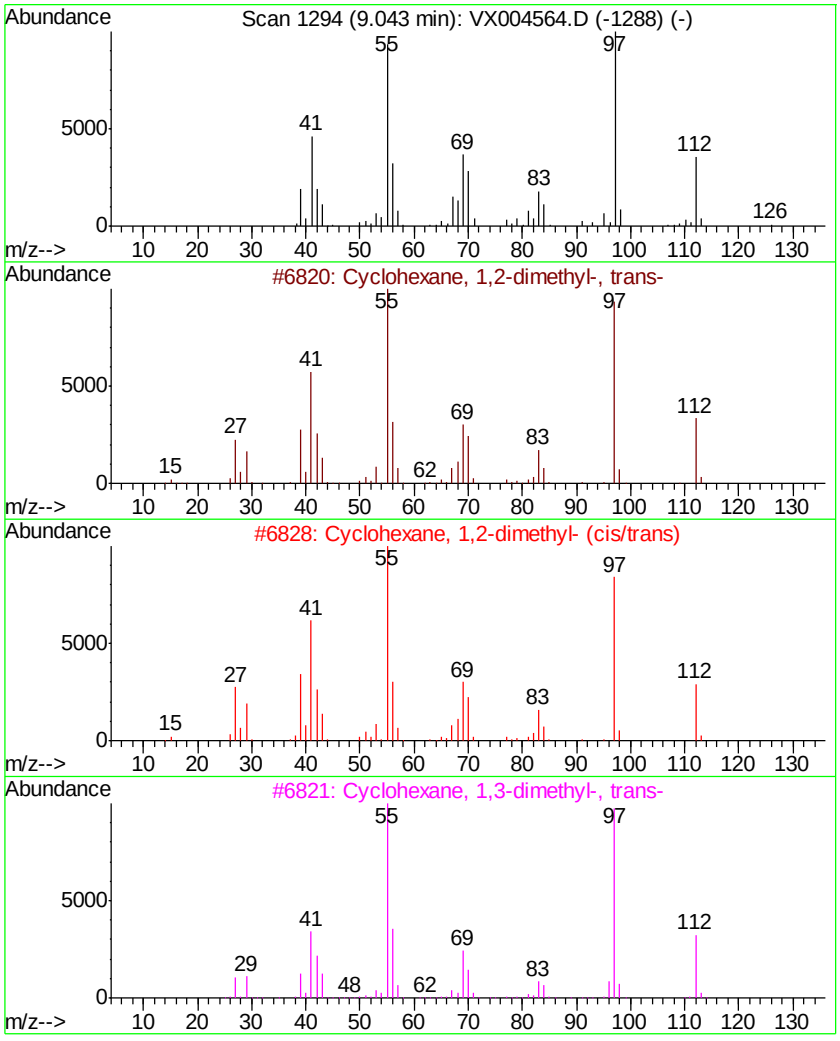
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

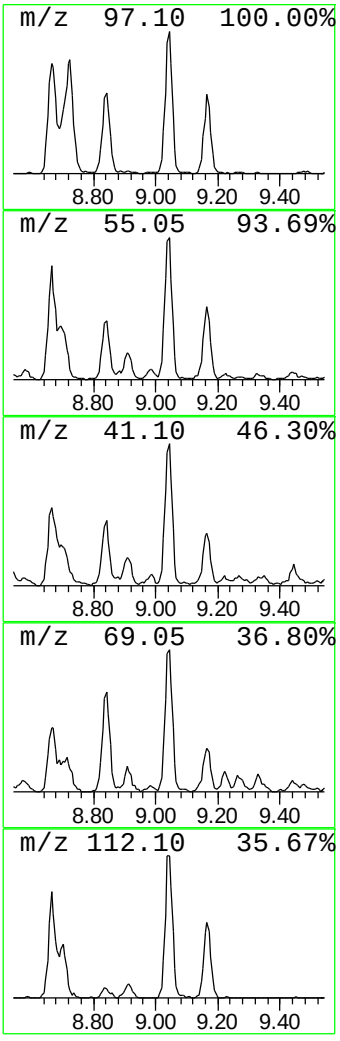
****

Peak Number 4 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.04	6.92 ug/l	132348	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	96
2	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	96
3	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	90
4	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	90
5	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	90





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

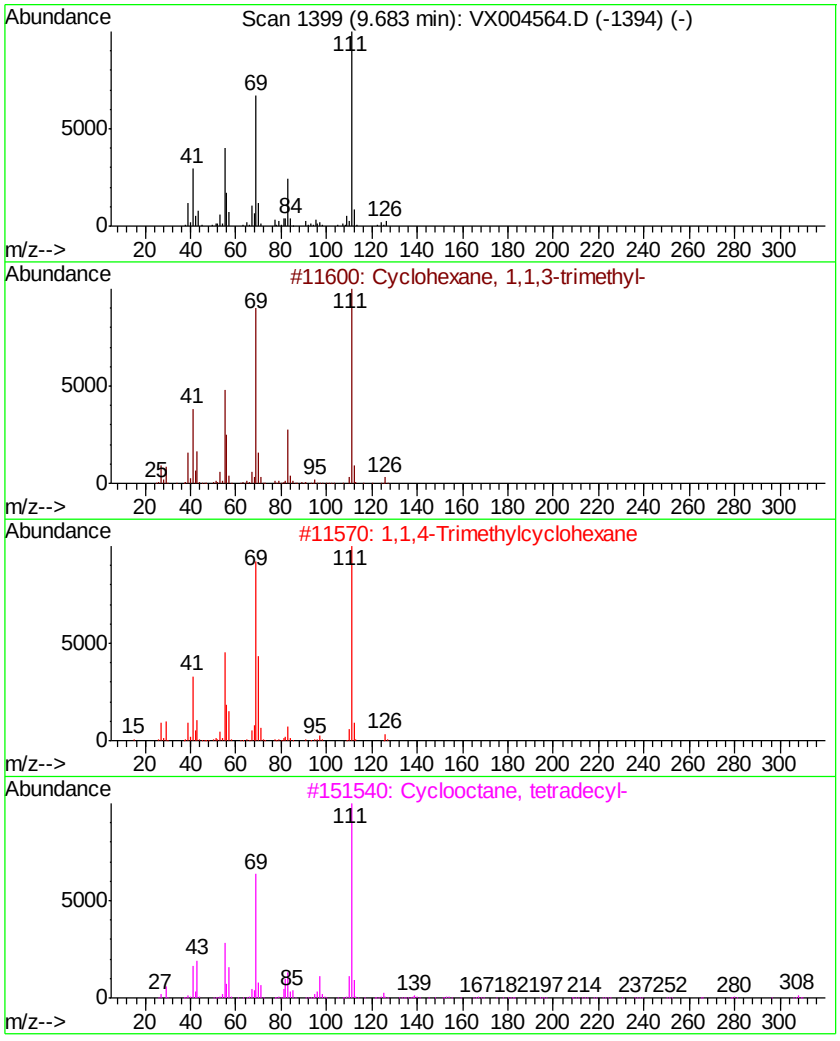
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

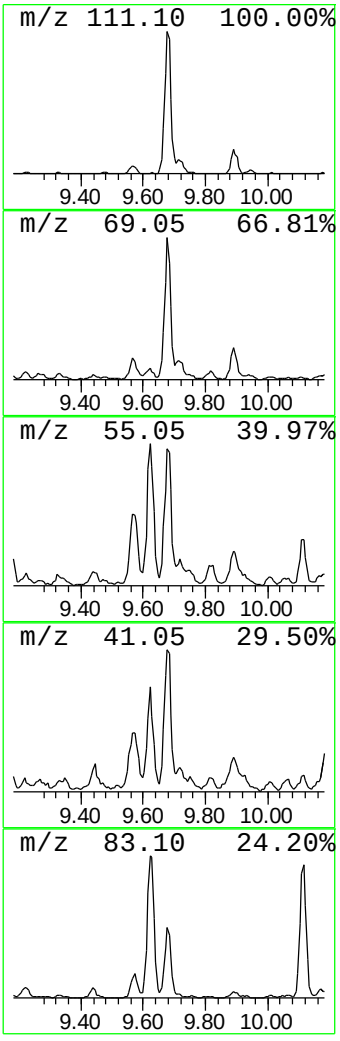
****

Peak Number 5 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.68	5.46 ug/l	104474	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	94
2	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	72
3	Cyclooctane, tetradecyl-	308	C22H44	149003-36-1	64
4	6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	64
5	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

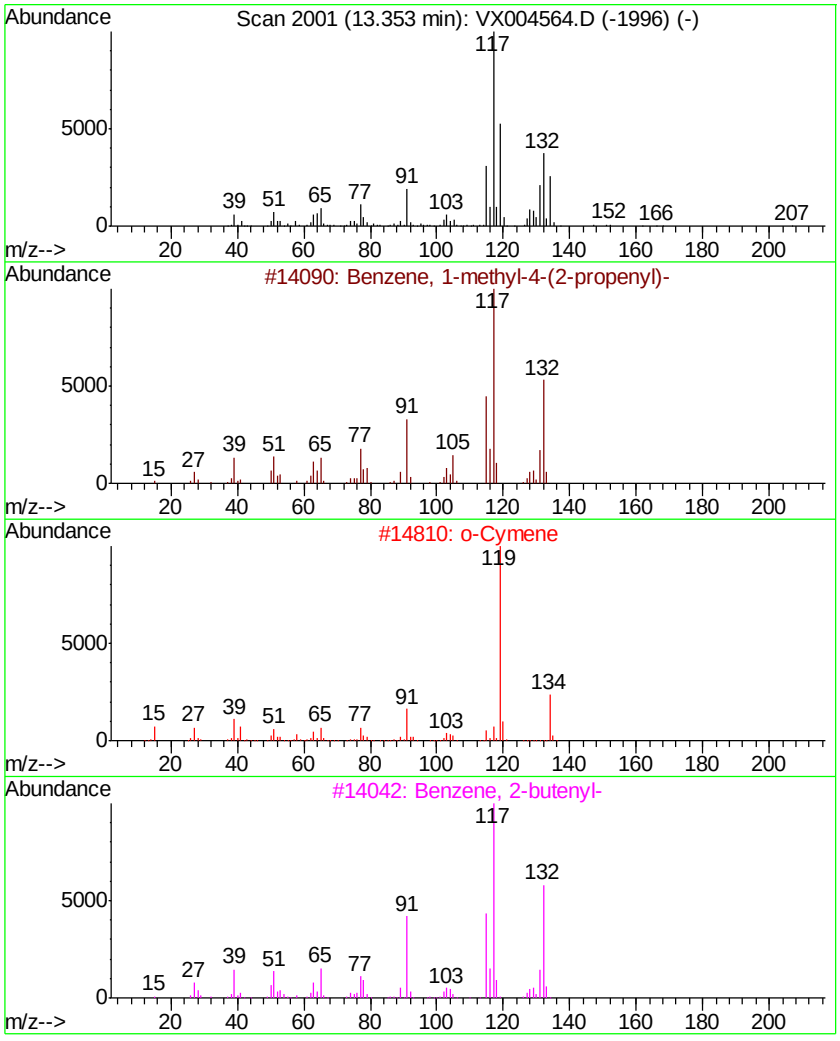
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

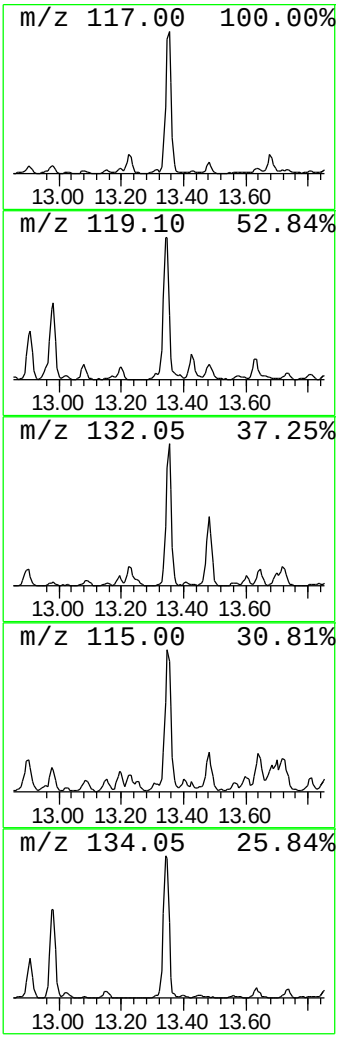
****

Peak Number 6 Benzene, 1-methyl-4-(2-prop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	11.72 ug/l	252568	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	64
2	o-Cymene	134	C10H14	000527-84-4	50
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	50
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	50
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091418\
Data File : VX004564.D
Acq On : 15 Sep 2018 05:23
Operator : JC/MD
Sample : J4925-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : S13-0254

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.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
Pentane, 3-methyl-	3.17	8.2	ug/l	131567	1	5.67	803391	50.0
Cyclopentane, met...	4.40	8.1	ug/l	130659	1	5.67	803391	50.0
Cyclopentane, 1,2...	6.45	5.4	ug/l	89695	2	6.86	832258	50.0
Cyclohexane, 1,2-...	9.04	6.9	ug/l	132348	3	10.12	956180	50.0
Cyclohexane, 1,1,...	9.68	5.5	ug/l	104474	3	10.12	956180	50.0
Benzene, 1-methyl...	13.35	11.7	ug/l	252568	4	12.08	1077450	50.0