LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100318\
Data File : VX004956.D
Acq On : 03 Oct 2018 09:19
Operator : JC/MD
Sample : J5084-04 10X
Misc : 4.21g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

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\82X092618W.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	5.500	696	713	722	rBV	182379	555063	2.98%	0.329%
2	5.665	733	740	745	rBV	208907	489670	2.63%	0.291%
3	5.915	771	781	795	rBV2	92141	265615	1.43%	0.158%
4	6.067	795	806	824	rBV3	196499	528932	2.84%	0.314%
5	6.348	841	852	862	rVB3	381166	1111536	5.97%	0.660%
6	6.860	927	936	944	rBV	398100	961781	5.16%	0.571%
7	7.457	1023	1034	1045	rBV4	123146	338304	1.82%	0.201%
8	7.573	1045	1053	1058	rBV2	91944	195545	1.05%	0.116%
9	7.634	1058	1063	1069	rBV	110791	217837	1.17%	0.129%
10	8.055	1122	1132	1144	rVB	465485	961548	5.16%	0.571%
11	8.177	1144	1152	1160	rBV2	433597	989315	5.31%	0.587%
12	8.256	1160	1165	1174	rVV2	200787	423081	2.27%	0.251%
13	8.341	1174	1179	1182	rVV	206038	345857	1.86%	0.205%
14	8.378	1182	1185	1192	rVB	120159	195881	1.05%	0.116%
15	8.500	1201	1205	1210	rBV	245377	405233	2.18%	0.241%
16	8.677	1226	1234	1236	rBV3	263428	472137	2.54%	0.280%
17	8.713	1236	1240	1246	rVB	918930	1483035	7.96%	0.880%
18	8.786	1246	1252	1258	rBV	1204489	1887420	10.13%	1.120%
19	8.884	1264	1268	1276	rVB2	79715	188720	1.01%	0.112%
20	8.975	1276	1283	1290	rBV3	244196	507946	2.73%	0.301%
21	9.561	1374	1379	1385	rBV2	193938	409835	2.20%	0.243%
22	9.963	1441	1445	1450	rVB	551075	776796	4.17%	0.461%
23	10.067	1457	1462	1466	rBV	489444	647062	3.47%	0.384%
24	10.115	1466	1470	1474	rVV	845944	1126202	6.05%	0.668%
25	10.256	1488	1493	1498	rBV	1910815	2619881	14.07%	1.555%
26	10.359	1504	1510	1516	rBV	9366316	12941202	69.49%	7.681%
27	10.414	1516	1519	1531	rVB2	653066	1316342	7.07%	0.781%
28	10.640	1552	1556	1560	rBV	309086	431044	2.31%	0.256%
29	10.701	1560	1566	1575	rVV	4352172	5925382	31.82%	3.517%
30	10.835	1580	1588	1592	rBV	267890	472702	2.54%	0.281%
31	10.914	1592	1601	1605	rBV4	196428	368484	1.98%	0.219%
32	11.018	1612	1618	1625	rBV	436511	678182	3.64%	0.403%
33	11.085	1625	1629	1632	rVV	255112	378000	2.03%	0.224%
34	11.140	1632	1638	1641	rVV	1289056	2094612	11.25%	1.243%

LSC Area Percent Report

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Operator : JC/MD
Sample : J5084-04 10X
Misc : 4.21g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

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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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Title : SW846 8260

35	11.170	1641	1643	1649	rVV2	835229	1223679	6.57%	0.726%
36	11.243	1649	1655	1659	rVV	516187	745921	4.01%	0.443%
37	11.359	1663	1674	1681	rVV	1583301	2480495	13.32%	1.472%
38	11.438	1681	1687	1694	rVV	9008894	15614220	83.84%	9.268%
39	11.505	1694	1698	1710	rVB	4191260	6704560	36.00%	3.980%
40	11.670	1720	1725	1732	rBV	3417572	4438859	23.84%	2.635%
41	11.810	1743	1748	1755	rVB	15303208	18623060	100.00%	11.054%
42	11.896	1759	1762	1764	rBV	149818	195373	1.05%	0.116%
43	11.944	1768	1770	1774	rVB	321472	370075	1.99%	0.220%
44	11.987	1774	1777	1780	rBV2	234983	330357	1.77%	0.196%
45	12.030	1780	1784	1787	rVB	587687	697657	3.75%	0.414%
46	12.079	1787	1792	1797	rBV3	1154204	1740454	9.35%	1.033%
47	12.146	1797	1803	1807	rBV	3645372	4741921	25.46%	2.815%
48	12.225	1814	1816	1823	rVB2	309113	413502	2.22%	0.245%
49	12.304	1823	1829	1831	rBV	3408518	4981444	26.75%	2.957%
50	12.322	1831	1832	1836	rVV	3075849	2912041	15.64%	1.728%
51	12.371	1836	1840	1847	rVB4	4193881	6786530	36.44%	4.028%
52	12.475	1847	1857	1861	rBV3	790469	1408548	7.56%	0.836%
53	12.524	1861	1865	1871	rVB2	1318088	1992838	10.70%	1.183%
54	12.591	1871	1876	1878	rBV	2117640	3049015	16.37%	1.810%
55	12.609	1878	1879	1884	rVV	2019949	1959374	10.52%	1.163%
56	12.670	1884	1889	1893	rVV	3709093	4447852	23.88%	2.640%
57	12.700	1893	1894	1899	rVV2	382967	441948	2.37%	0.262%
58	12.761	1899	1904	1913	rVB2	1090535	2390470	12.84%	1.419%
59	12.853	1914	1919	1924	rBV4	180092	293628	1.58%	0.174%
60	12.908	1924	1928	1932	rVB	758622	944854	5.07%	0.561%
61	12.981	1932	1940	1943	rBV	1850211	2674924	14.36%	1.588%
62	13.017	1943	1946	1952	rVB	2682105	3335120	17.91%	1.980%
63	13.078	1952	1956	1958	rBV	561814	757538	4.07%	0.450%
64	13.103	1958	1960	1962	rVV	692970	800604	4.30%	0.475%
65	13.127	1962	1964	1967	rVB	518559	512386	2.75%	0.304%
66	13.225	1973	1980	1984	rVB3	1611392	2489749	13.37%	1.478%
67	13.267	1984	1987	1990	rVB2	464536	508779	2.73%	0.302%
68	13.316	1990	1995	1997	rBV3	737320	1092711	5.87%	0.649%
69	13.353	1997	2001	2006	rVB2	2662294	3666342	19.69%	2.176%
70	13.426	2011	2013	2018	rVB	605730	682459	3.66%	0.405%
71	13.481	2018	2022	2031	rVB2	557377	851443	4.57%	0.505%

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ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Title : SW846 8260

72	13.560	2031	2035	2038	rBV2	354188	509913	2.74%	0.303%
73	13.603	2038	2042	2045	rBV	535411	682587	3.67%	0.405%
74	13.639	2045	2048	2054	rVB2	847669	1480856	7.95%	0.879%
75	13.725	2059	2062	2067	rVB3	537095	906551	4.87%	0.538%
76	13.834	2075	2080	2086	rVB	2297642	2900753	15.58%	1.722%
77	13.920	2091	2094	2098	rVB3	237240	347637	1.87%	0.206%
78	13.987	2098	2105	2109	rBV4	472867	894578	4.80%	0.531%
79	14.029	2109	2112	2115	rVV	260666	296883	1.59%	0.176%
80	14.090	2119	2122	2125	rVB3	248737	303390	1.63%	0.180%
81	14.133	2125	2129	2133	rBV	692167	829573	4.45%	0.492%
82	14.273	2148	2152	2157	rBV	668493	1015486	5.45%	0.603%
83	14.383	2166	2170	2175	rBV	366658	533332	2.86%	0.317%
84	14.432	2175	2178	2182	rVB	488546	556495	2.99%	0.330%
85	14.548	2191	2197	2201	rBV4	139679	283570	1.52%	0.168%
86	14.700	2212	2222	2227	rBV	3002632	3907520	20.98%	2.319%
87	14.785	2232	2236	2239	rBV	133278	186532	1.00%	0.111%
88	14.840	2241	2245	2254	rVB	1420292	1863783	10.01%	1.106%
89	15.444	2337	2344	2348	rBV	121068	194294	1.04%	0.115%
90	15.553	2356	2362	2372	rVB	233212	408117	2.19%	0.242%
91	15.688	2379	2384	2388	rBV	230266	360381	1.94%	0.214%

Sum of corrected areas: 168473143

LSC Report - Integrated Chromatogram

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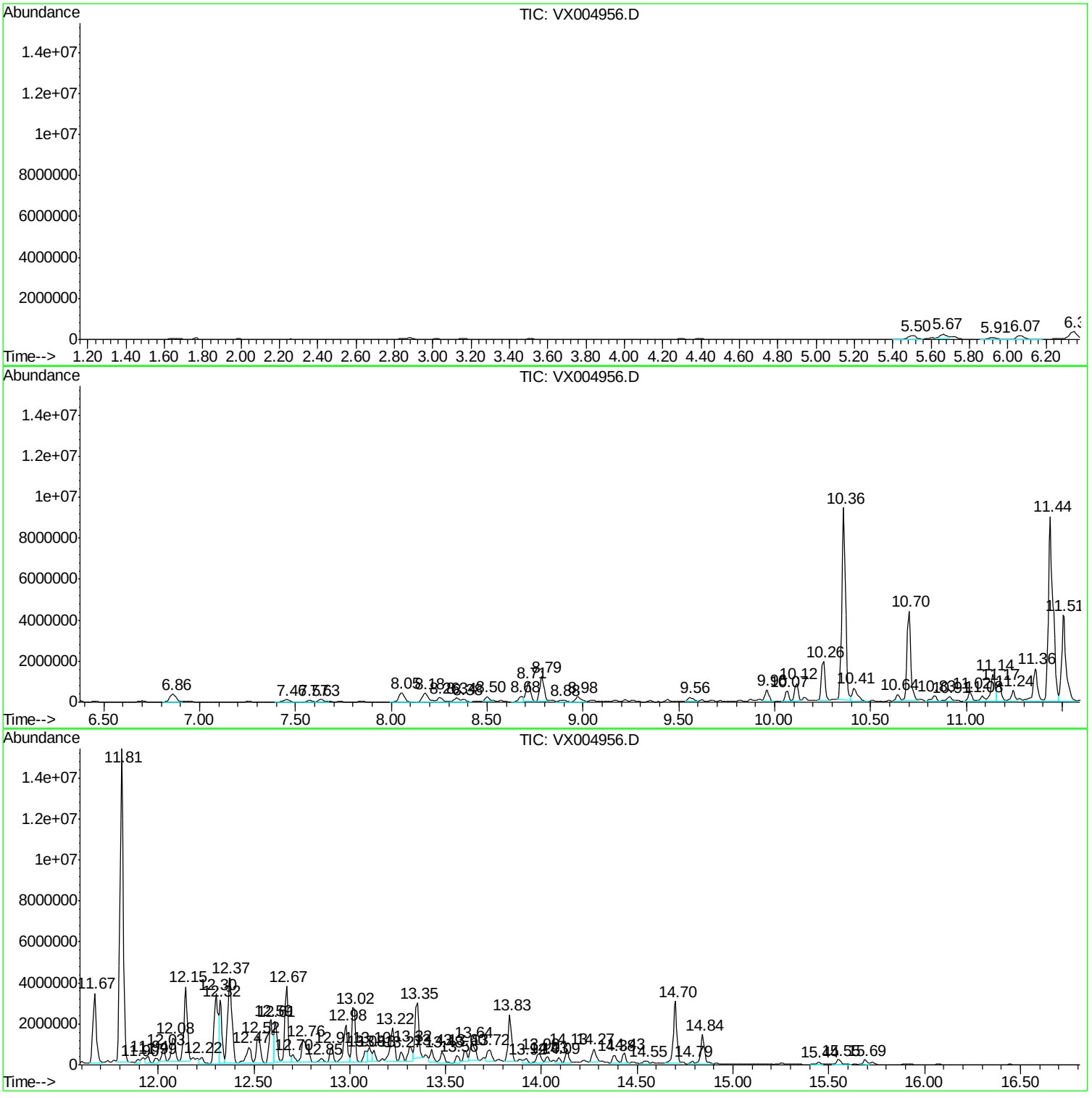
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.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\VX100318\
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ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

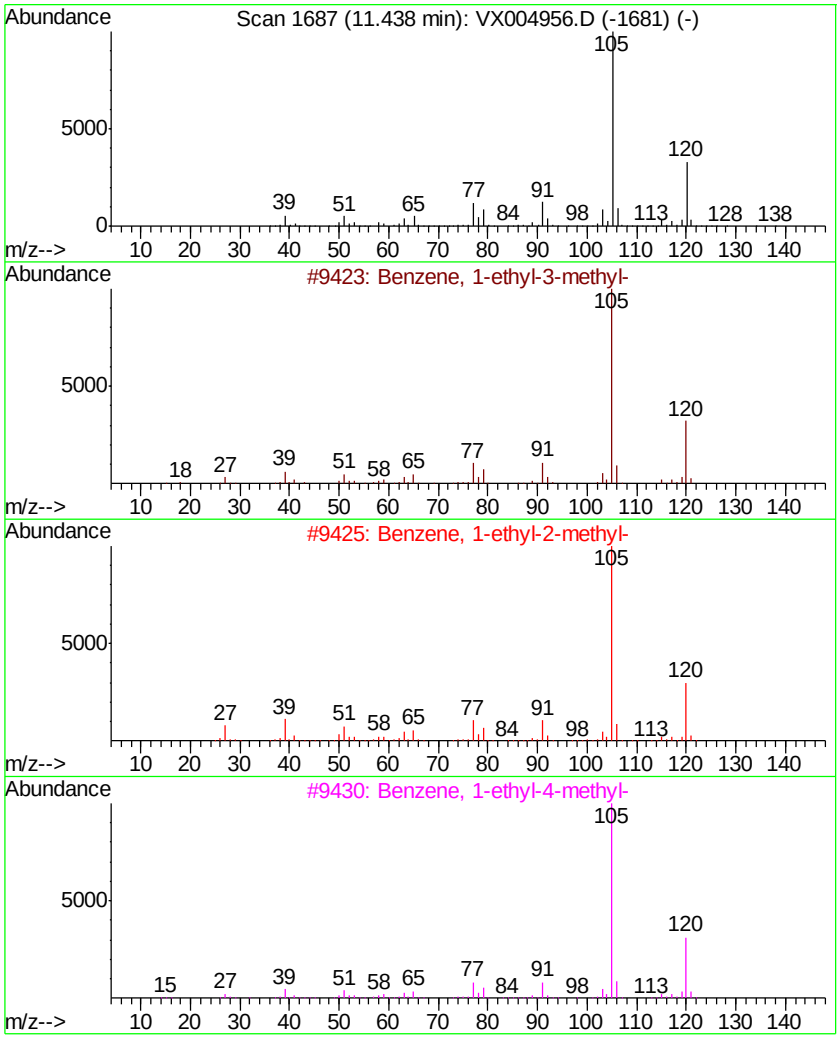
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

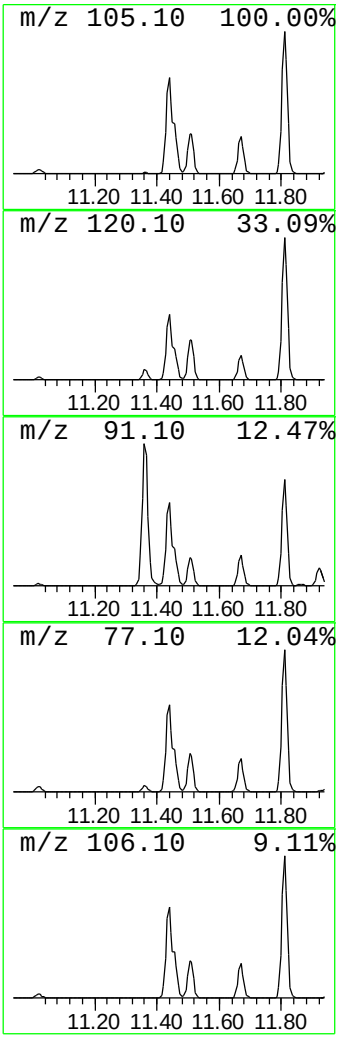
****

Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	448.57 ug/l	15614200	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100318\
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Operator : JC/MD
Sample : J5084-04 10X
Misc : 4.21g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

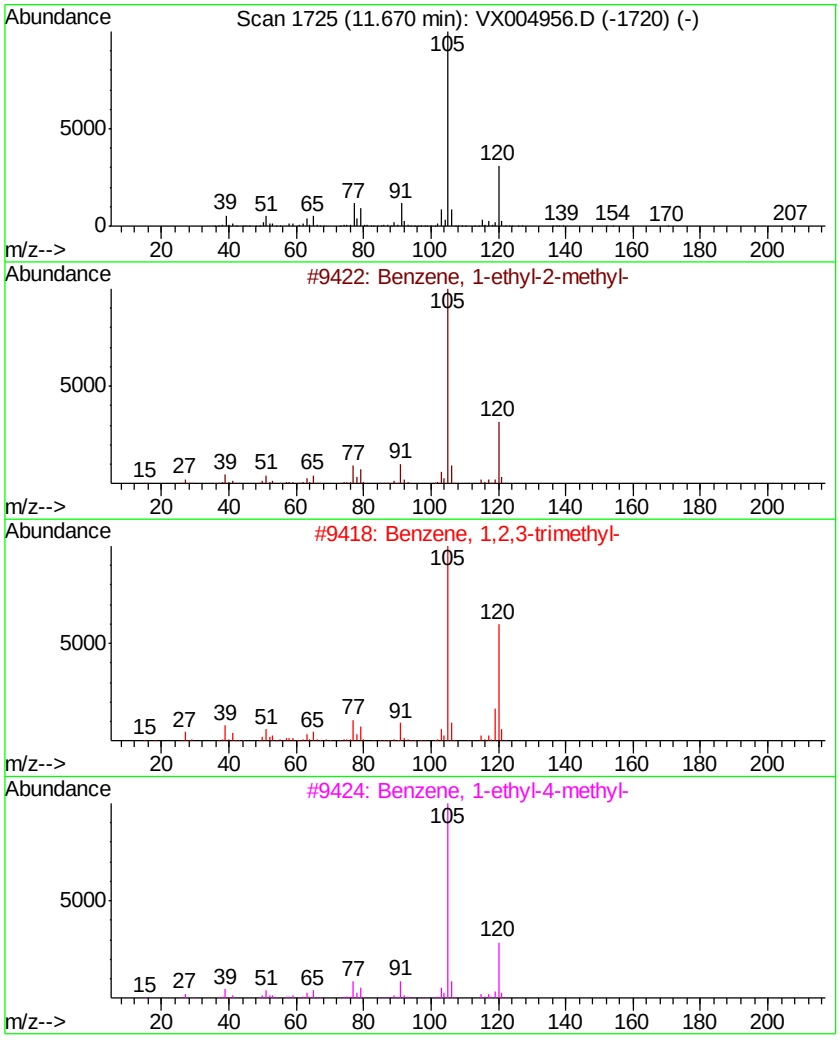
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

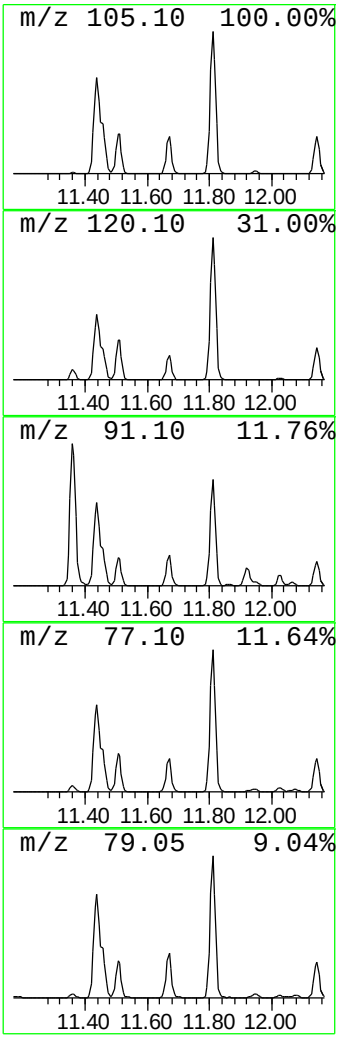
****

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	127.52 ug/l	4438860	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Mesitylene	120	C9H12	000108-67-8	91





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100318\
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ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

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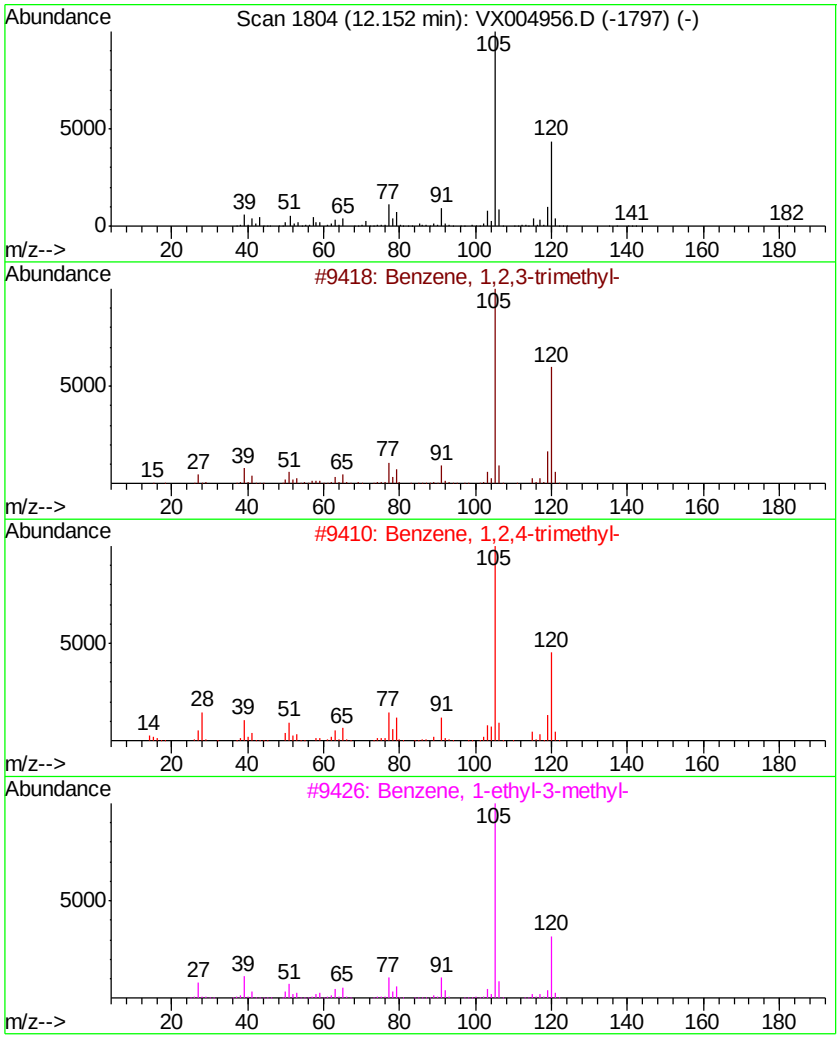
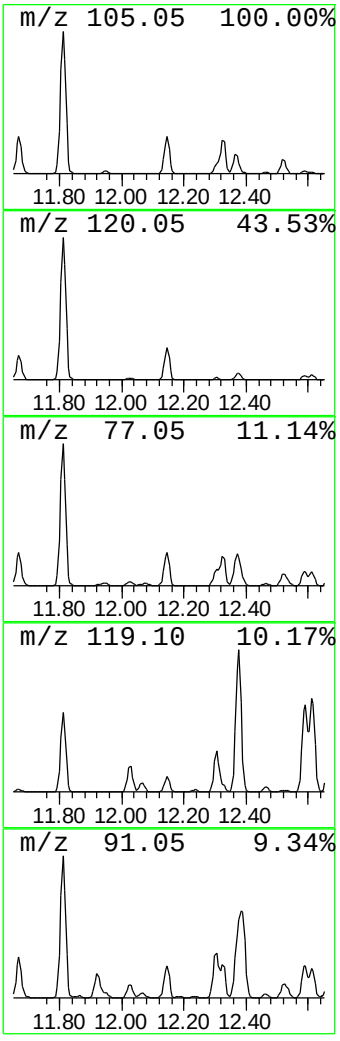
Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	136.23 ug/l	4741920	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5	Mesitylene	120	C9H12	000108-67-8	87





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ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

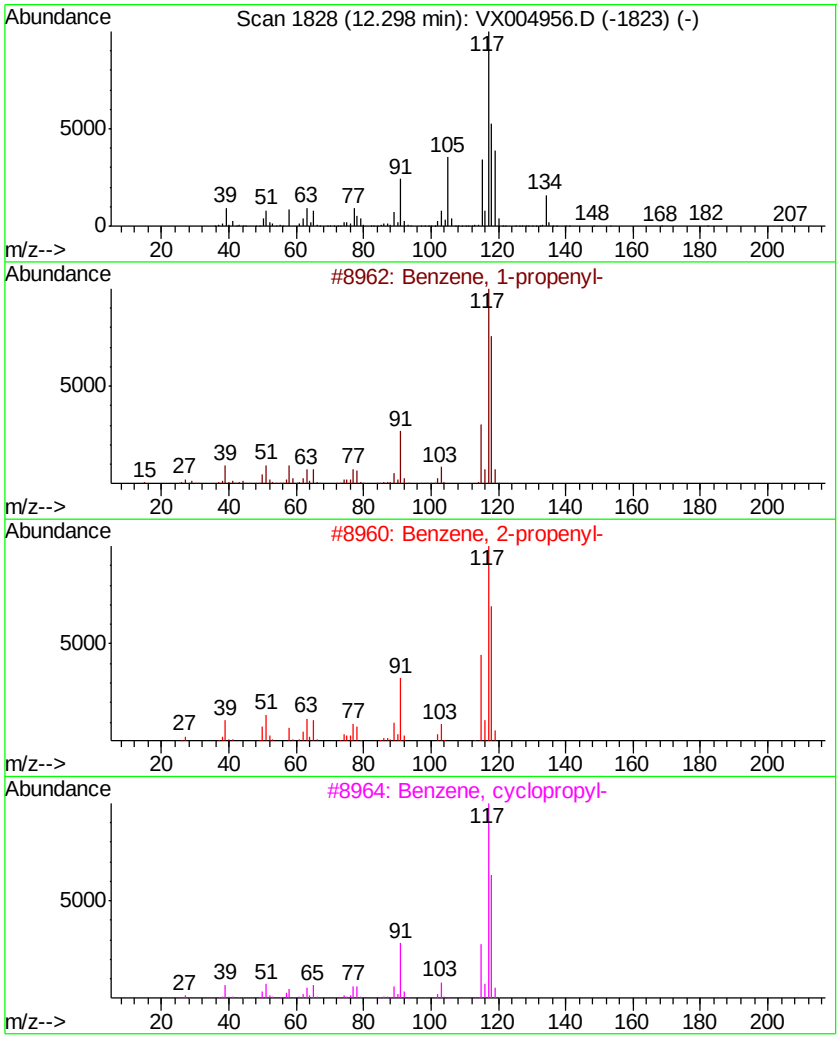
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

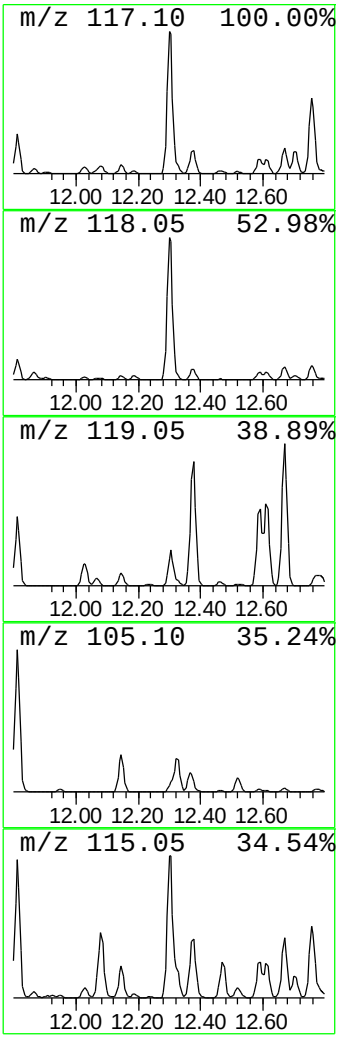
****

Peak Number 4 Benzene, 1-propenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	143.11 ug/l	4981440	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	90
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
5	Indane	118	C9H10	000496-11-7	49





Library Search Compound Report

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ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

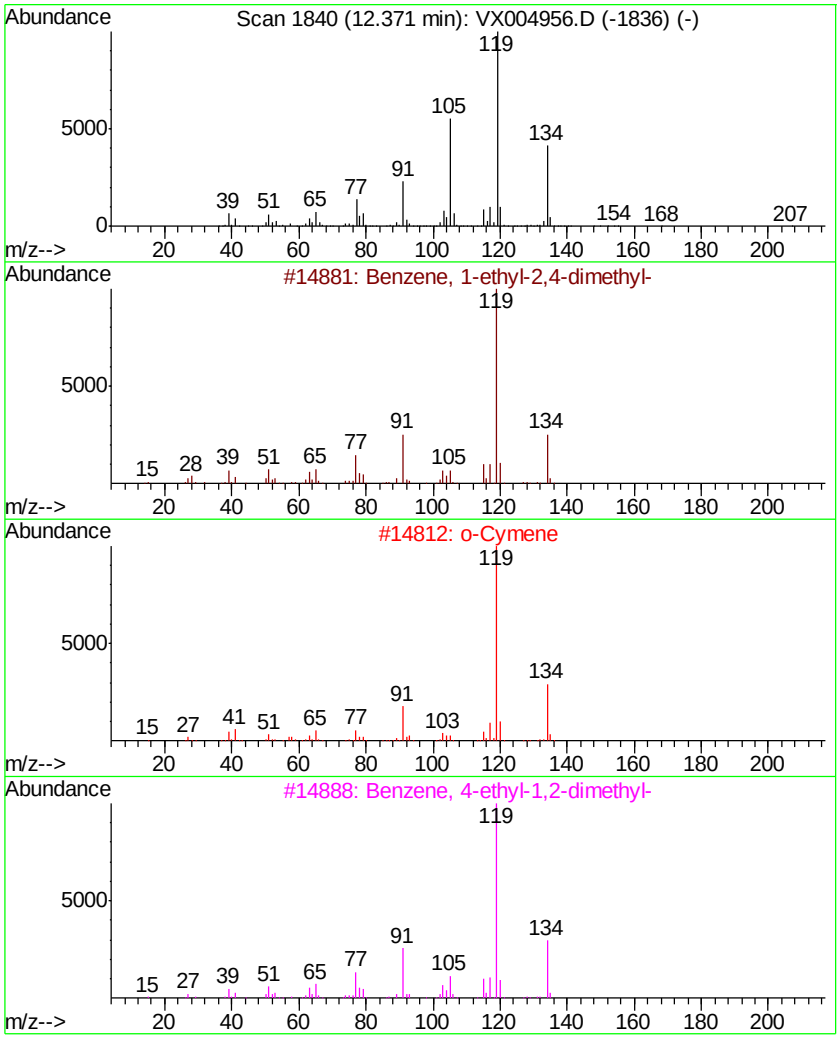
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

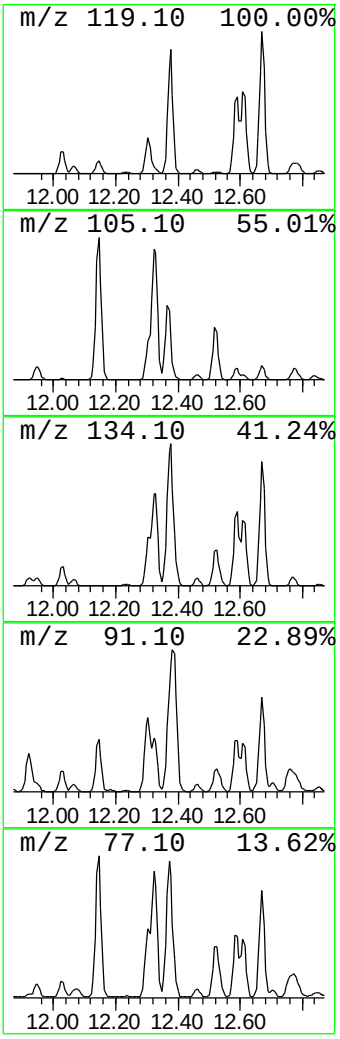
****

Peak Number 5 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	194.96 ug/l	6786530	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
2	o-Cymene	134	C10H14	000527-84-4	94
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94
4	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	93
5	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	93





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100318\
Data File : VX004956.D
Acq On : 03 Oct 2018 09:19
Operator : JC/MD
Sample : J5084-04 10X
Misc : 4.21g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

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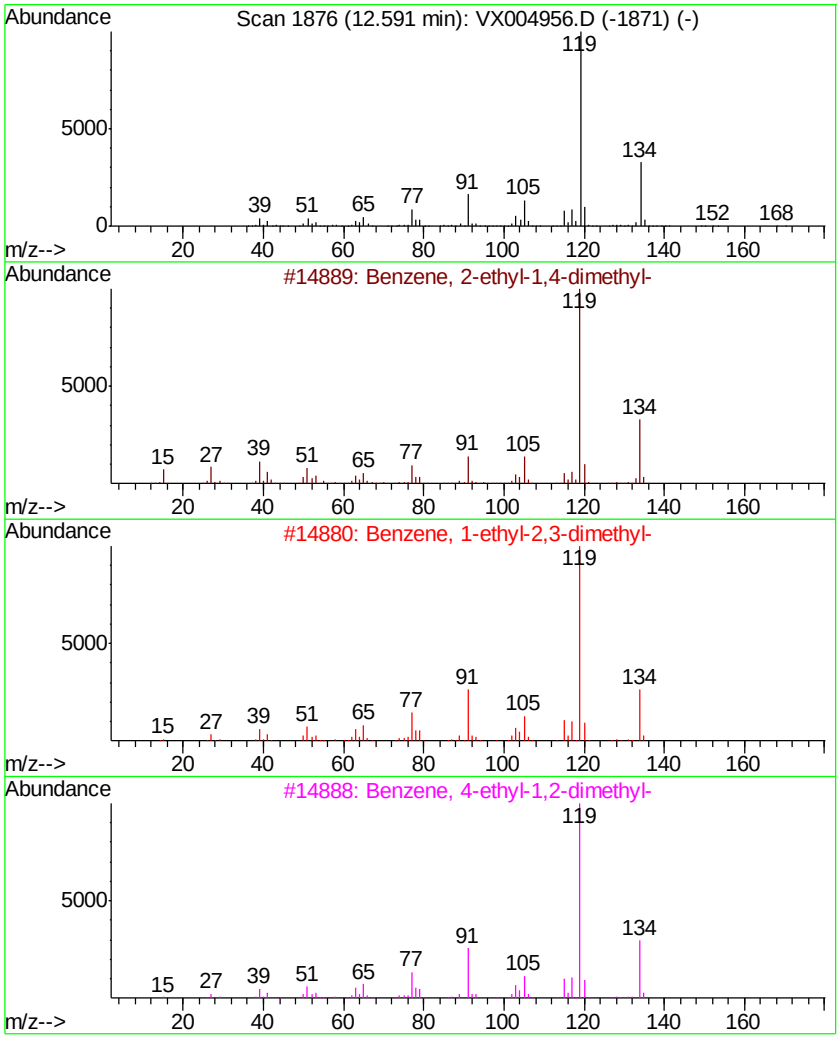
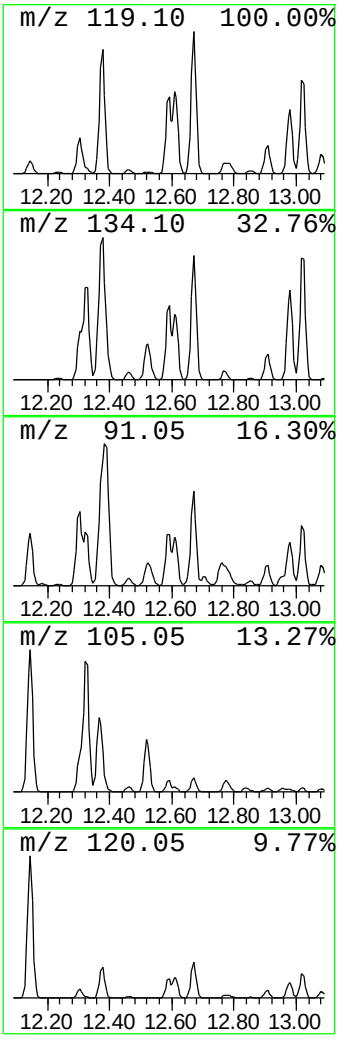
Peak Number 6 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.59	87.59 ug/l	3049020	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94
5	o-Cymene	134	C10H14	000527-84-4	94





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100318\
Data File : VX004956.D
Acq On : 03 Oct 2018 09:19
Operator : JC/MD
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Misc : 4.21g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

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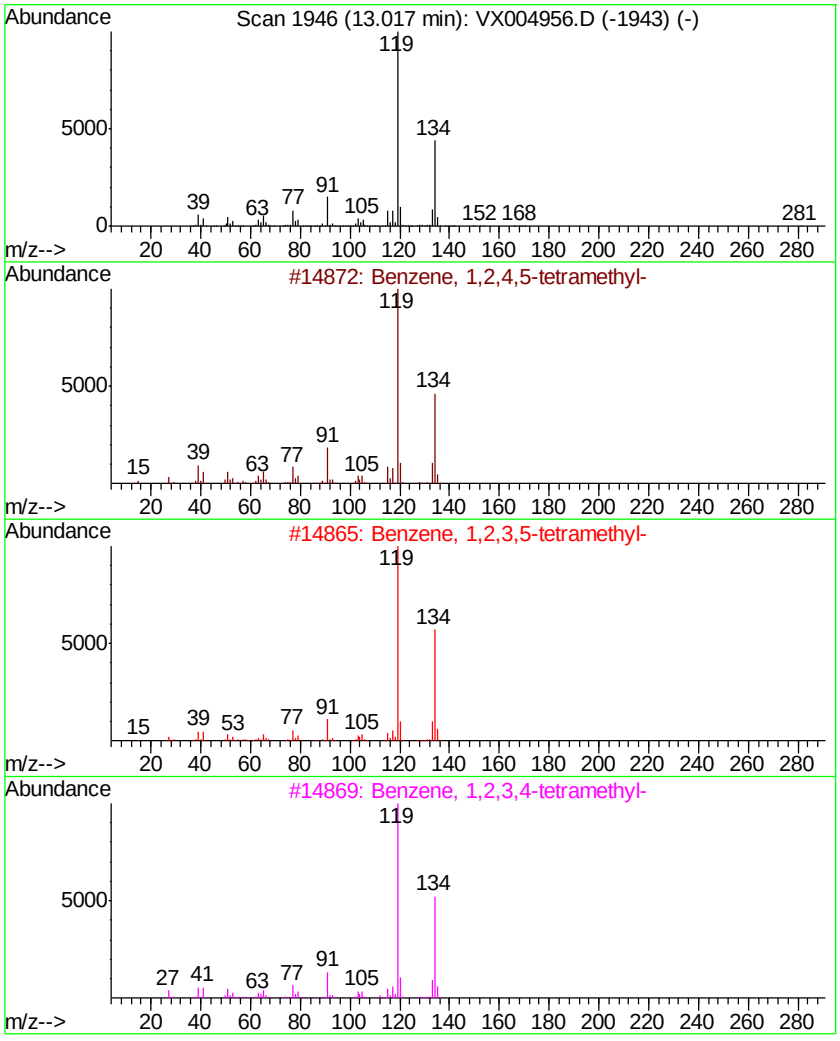
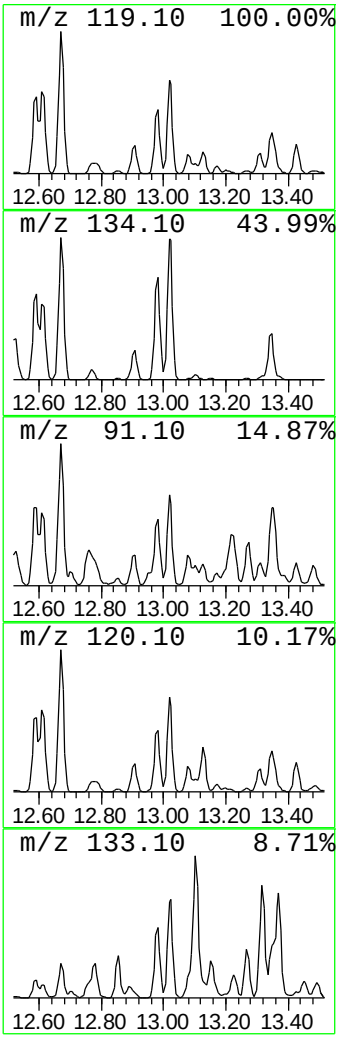
Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	95.81 ug/l	3335120	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5	o-Cymene	134	C10H14	000527-84-4	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100318\
Data File : VX004956.D
Acq On : 03 Oct 2018 09:19
Operator : JC/MD
Sample : J5084-04 10X
Misc : 4.21g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

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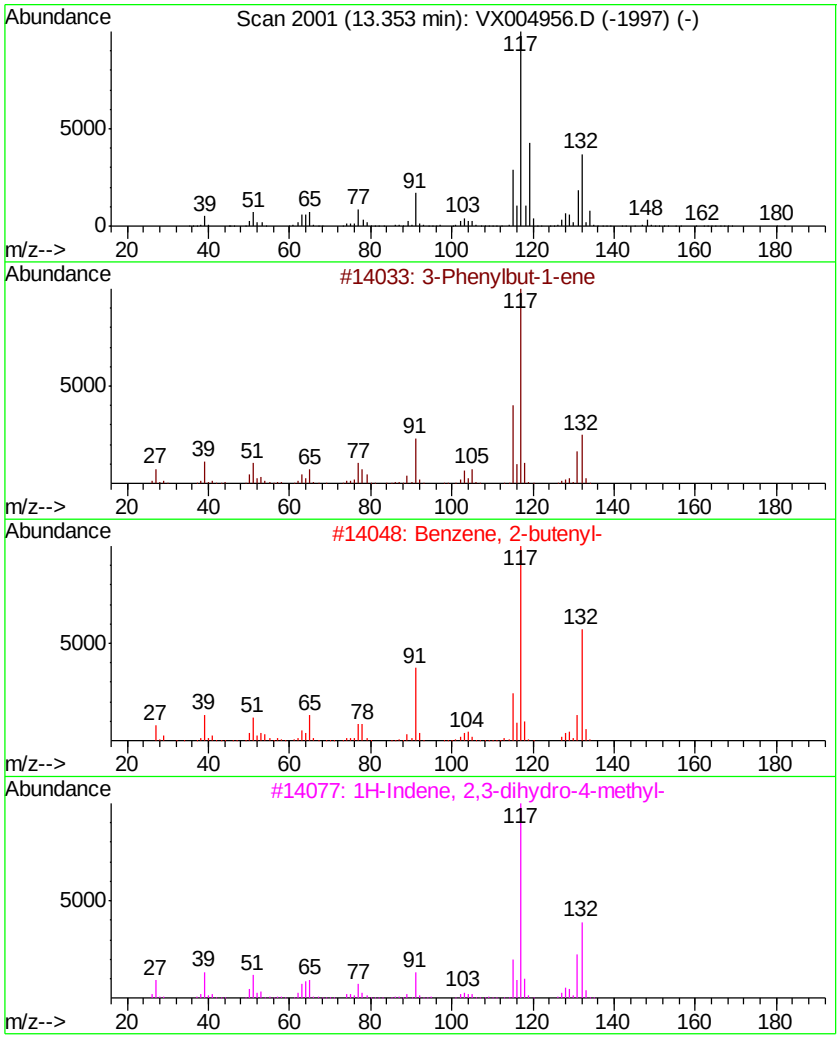
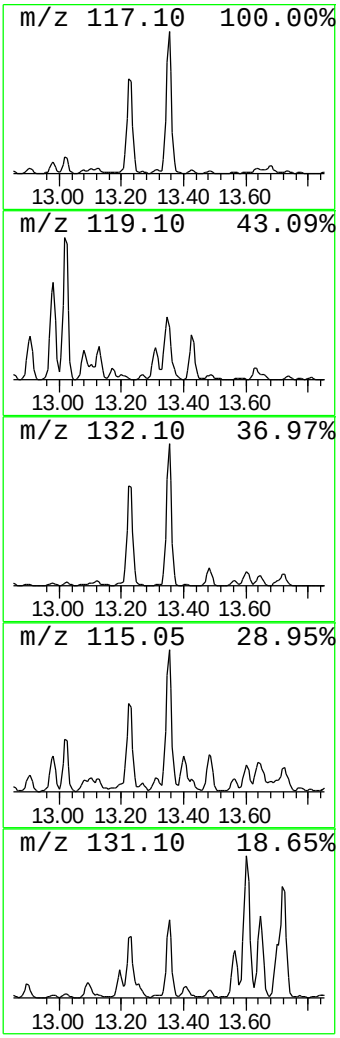
Peak Number 9 3-Phenylbut-1-ene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	105.33 ug/l	3666340	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	76
2	Benzene, 2-butenyl-	132	C10H12	001560-06-1	76
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	70
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
5	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100318\
Data File : VX004956.D
Acq On : 03 Oct 2018 09:19
Operator : JC/MD
Sample : J5084-04 10X
Misc : 4.21g/5mL/100uL/5.0mL/MSVOA_X/MEOH
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Instrument : MSVOA_X
ClientSampleId : B-7(6-6.5)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.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
Benzene, 1-ethyl-...	11.44	448.6	ug/l	15614200	4	12.08	1740450	50.0
Benzene, 1-ethyl-...	11.67	127.5	ug/l	4438860	4	12.08	1740450	50.0
Benzene, 1,2,3-tr...	12.15	136.2	ug/l	4741920	4	12.08	1740450	50.0
Benzene, 1-propenyl-	12.30	143.1	ug/l	4981440	4	12.08	1740450	50.0
Benzene, 1-ethyl-...	12.37	195.0	ug/l	6786530	4	12.08	1740450	50.0
Benzene, 2-ethyl-...	12.59	87.6	ug/l	3049020	4	12.08	1740450	50.0
Benzene, 1,2,4,5-...	13.02	95.8	ug/l	3335120	4	12.08	1740450	50.0
3-Phenylbut-1-ene	13.35	105.3	ug/l	3666340	4	12.08	1740450	50.0