LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SFAMXLM112221WMA.M
Title : VOC Analysis

Signal : TIC: VX025656.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	54	rVB	29761	35619	0.63%	0.368%
2	1.648	89	92	98	rVB	22548	27299	0.48%	0.282%
3	2.282	190	196	205	rBV	56680	92986	1.64%	0.962%
4	2.953	300	306	311	rBV4	2204	4746	0.08%	0.049%
5	3.081	323	327	337	rVB2	4042	8555	0.15%	0.088%
6	3.428	380	384	390	rVV4	1570	2822	0.05%	0.029%
7	4.190	505	509	512	rBV3	528	1076	0.02%	0.011%
8	4.288	517	525	537	rVB3	6845	19861	0.35%	0.205%
9	4.489	548	558	586	rBV	19643	89056	1.57%	0.921%
10	5.062	642	652	669	rVB	43886	145952	2.58%	1.509%
11	5.465	709	718	730	rVV4	8911	30419	0.54%	0.315%
12	5.824	769	777	784	rBV5	2776	8364	0.15%	0.086%
13	5.971	790	801	816	rBV2	113178	329816	5.83%	3.411%
14	6.147	824	830	840	rVB5	2959	8206	0.15%	0.085%
15	6.251	840	847	855	rVB6	2785	7532	0.13%	0.078%
16	6.355	855	864	875	rBV6	6377	19138	0.34%	0.198%
17	6.605	899	905	916	rVB6	2608	6339	0.11%	0.066%
18	6.763	921	931	943	rBV	121913	315345	5.57%	3.261%
19	7.129	980	991	1013	rBV	2567738	5657985	100.00%	58.508%
20	7.312	1014	1021	1027	rBV	67070	152302	2.69%	1.575%
21	7.476	1044	1048	1049	rBV2	716	808	0.01%	0.008%
22	7.653	1072	1077	1084	rVB4	2611	5359	0.09%	0.055%
23	7.769	1090	1096	1103	rBV4	3292	6506	0.11%	0.067%
24	7.958	1120	1127	1132	rVV4	3537	6725	0.12%	0.070%
25	8.190	1160	1165	1168	rVV3	1071	1888	0.03%	0.020%
26	8.226	1168	1171	1174	rVV4	1141	1858	0.03%	0.019%
27	8.275	1174	1179	1182	rVV2	4444	7384	0.13%	0.076%
28	8.330	1182	1188	1198	rVV	43605	82896	1.47%	0.857%
29	8.440	1202	1206	1211	rVB4	1687	2926	0.05%	0.030%
30	8.598	1226	1232	1234	rBV2	6872	10228	0.18%	0.106%
31	8.653	1235	1241	1248	rVB	146542	251817	4.45%	2.604%
32	8.720	1248	1252	1258	rBV	16179	25724	0.45%	0.266%
33	8.818	1265	1268	1270	rBV2	1432	1680	0.03%	0.017%
34	8.909	1279	1283	1286	rBV2	5500	7819	0.14%	0.081%
35	8.958	1286	1291	1300	rVB2	30223	61085	1.08%	0.632%
36	9.098	1310	1314	1320	rBV3	1753	3052	0.05%	0.032%

LSC Area Percent Report

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Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SFAMXLM112221WMA.M
Title : VOC Analysis

37	9.202	1329	1331	1337	rBV5	551	989	0.02%	0.010%
38	9.275	1337	1343	1350	rVV	107386	160721	2.84%	1.662%
39	9.397	1357	1363	1376	rBV	121158	194019	3.43%	2.006%
40	9.561	1386	1390	1395	rVB	8498	12224	0.22%	0.126%
41	9.616	1395	1399	1404	rBV2	8430	13972	0.25%	0.144%
42	9.702	1412	1413	1418	rVB2	977	1293	0.02%	0.013%
43	9.763	1418	1423	1428	rBV3	1241	1736	0.03%	0.018%
44	9.817	1428	1432	1440	rBV3	5890	10456	0.18%	0.108%
45	9.909	1443	1447	1452	rVB3	3143	4264	0.08%	0.044%
46	10.012	1459	1464	1466	rBV	1770	2421	0.04%	0.025%
47	10.061	1466	1472	1479	rBV	255796	375382	6.63%	3.882%
48	10.201	1490	1495	1501	rVB	6693	10091	0.18%	0.104%
49	10.305	1502	1512	1517	rVV	35753	56462	1.00%	0.584%
50	10.360	1517	1521	1529	rVB2	10492	14587	0.26%	0.151%
51	10.592	1551	1559	1563	rVV5	2828	4764	0.08%	0.049%
52	10.647	1563	1568	1577	rVB	36144	49019	0.87%	0.507%
53	10.781	1581	1590	1594	rBV4	7924	14746	0.26%	0.152%
54	10.860	1594	1603	1606	rBV2	6254	9900	0.17%	0.102%
55	10.896	1606	1609	1615	rVB2	5960	8171	0.14%	0.084%
56	10.970	1615	1621	1625	rBV	7100	9594	0.17%	0.099%
57	11.037	1628	1632	1636	rVB4	2443	4006	0.07%	0.041%
58	11.195	1653	1658	1667	rVB	150488	202333	3.58%	2.092%
59	11.311	1672	1677	1681	rBV	9454	13227	0.23%	0.137%
60	11.384	1685	1689	1695	rVV2	10368	15857	0.28%	0.164%
61	11.457	1698	1701	1702	rVV	5664	6812	0.12%	0.070%
62	11.476	1702	1704	1709	rVB	12354	14732	0.26%	0.152%
63	11.616	1722	1727	1735	rVB	7732	11039	0.20%	0.114%
64	11.683	1735	1738	1740	rBV2	764	1066	0.02%	0.011%
65	11.719	1740	1744	1746	rBV	7186	8781	0.16%	0.091%
66	11.756	1746	1750	1759	rVB	25208	33190	0.59%	0.343%
67	11.872	1761	1769	1770	rBV4	2129	3782	0.07%	0.039%
68	11.945	1778	1781	1783	rBV3	2349	2661	0.05%	0.028%
69	12.024	1789	1794	1800	rBV	319836	389504	6.88%	4.028%
70	12.091	1801	1805	1813	rVB2	12555	18333	0.32%	0.190%
71	12.268	1832	1834	1837	rVB	3325	3579	0.06%	0.037%
72	12.323	1838	1843	1850	rVB	226838	289799	5.12%	2.997%
73	12.427	1855	1860	1864	rBV	15693	18937	0.33%	0.196%
74	12.463	1864	1866	1873	rVB2	3165	4574	0.08%	0.047%
75	12.530	1874	1877	1880	rBV2	2800	4025	0.07%	0.042%
76	12.683	1900	1902	1905	rBV3	838	1120	0.02%	0.012%

LSC Area Percent Report

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Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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\SFAMXLM112221WMA.M
Title : VOC Analysis

77	12.719	1905	1908	1913	rVB3	3146	5102	0.09%	0.053%
78	12.768	1913	1916	1920	rBV3	1731	2190	0.04%	0.023%
79	12.896	1932	1937	1939	rBV4	2542	3968	0.07%	0.041%
80	12.969	1946	1949	1954	rVB4	4016	6011	0.11%	0.062%
81	13.042	1955	1961	1964	rBV4	1391	2637	0.05%	0.027%
82	13.268	1994	1998	2006	rVB4	13730	19806	0.35%	0.205%
83	13.384	2013	2017	2022	rBV2	5931	7431	0.13%	0.077%
84	13.579	2046	2049	2054	rVB5	1979	2450	0.04%	0.025%
85	13.628	2054	2057	2062	rBV4	1501	2626	0.05%	0.027%
86	13.780	2077	2082	2087	rVB	37769	50061	0.88%	0.518%
87	13.847	2089	2093	2097	rVB2	8047	10015	0.18%	0.104%
88	14.036	2121	2124	2128	rBV	9968	10886	0.19%	0.113%
89	14.103	2133	2135	2138	rVB4	2204	2497	0.04%	0.026%
90	14.506	2197	2201	2207	rVB7	2265	4408	0.08%	0.046%
91	14.640	2215	2223	2227	rBV	28134	37624	0.66%	0.389%
92	14.780	2239	2246	2252	rVB2	24902	37781	0.67%	0.391%
93	14.841	2254	2256	2260	rVB5	1426	1688	0.03%	0.017%
94	14.932	2269	2271	2278	rBV4	634	1424	0.03%	0.015%
95	15.182	2307	2312	2314	rBV5	1148	1900	0.03%	0.020%
96	15.213	2314	2317	2322	rVB3	3084	4142	0.07%	0.043%
97	15.347	2336	2339	2340	rBV3	634	741	0.01%	0.008%
98	15.493	2357	2363	2371	rVB6	2772	5564	0.10%	0.058%
99	15.615	2379	2383	2386	rBV4	3377	5055	0.09%	0.052%
100	16.164	2468	2473	2477	rBV2	669	1046	0.02%	0.011%

Sum of corrected areas: 9670394

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
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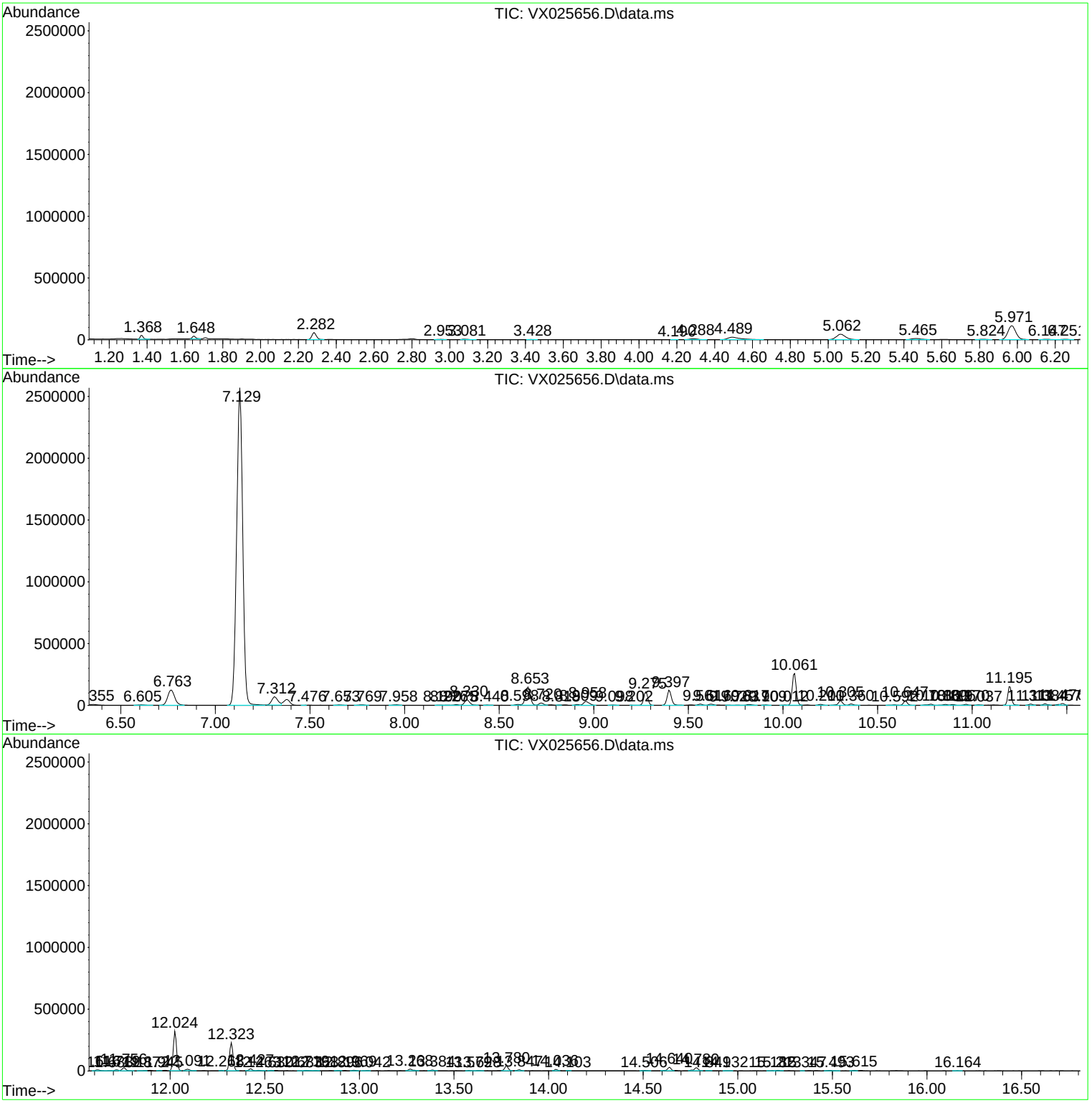
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
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Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

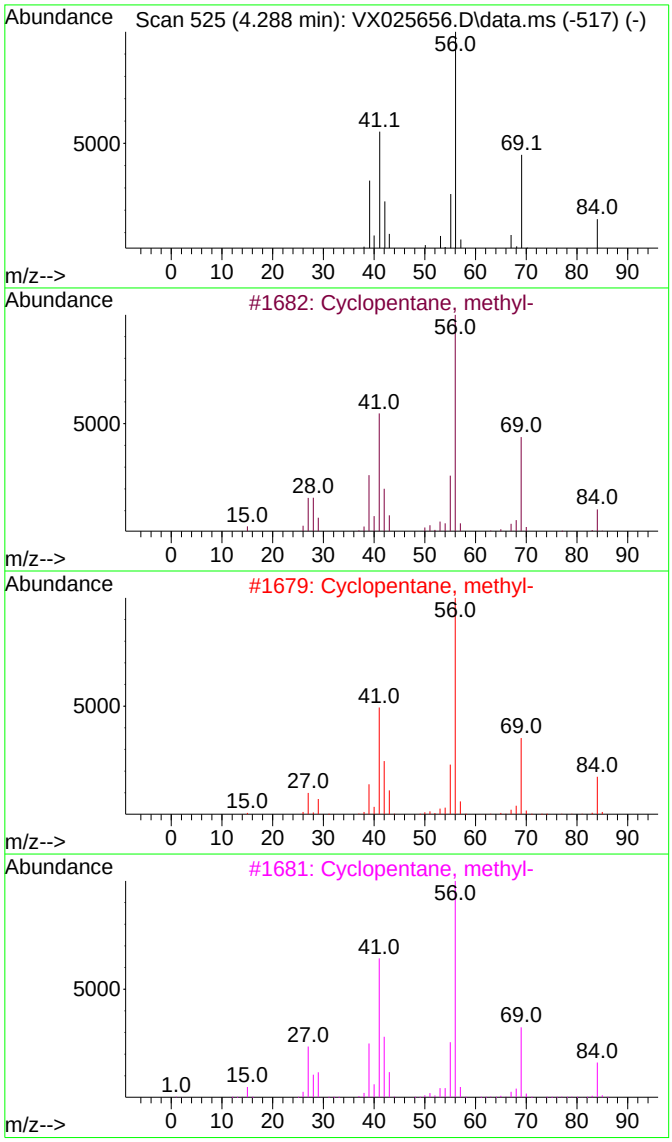
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

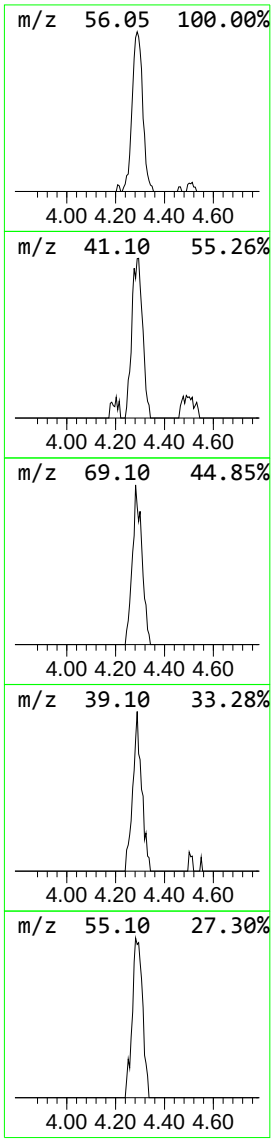
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Cyclic4.288 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.288	3.15 ug/L	19861	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

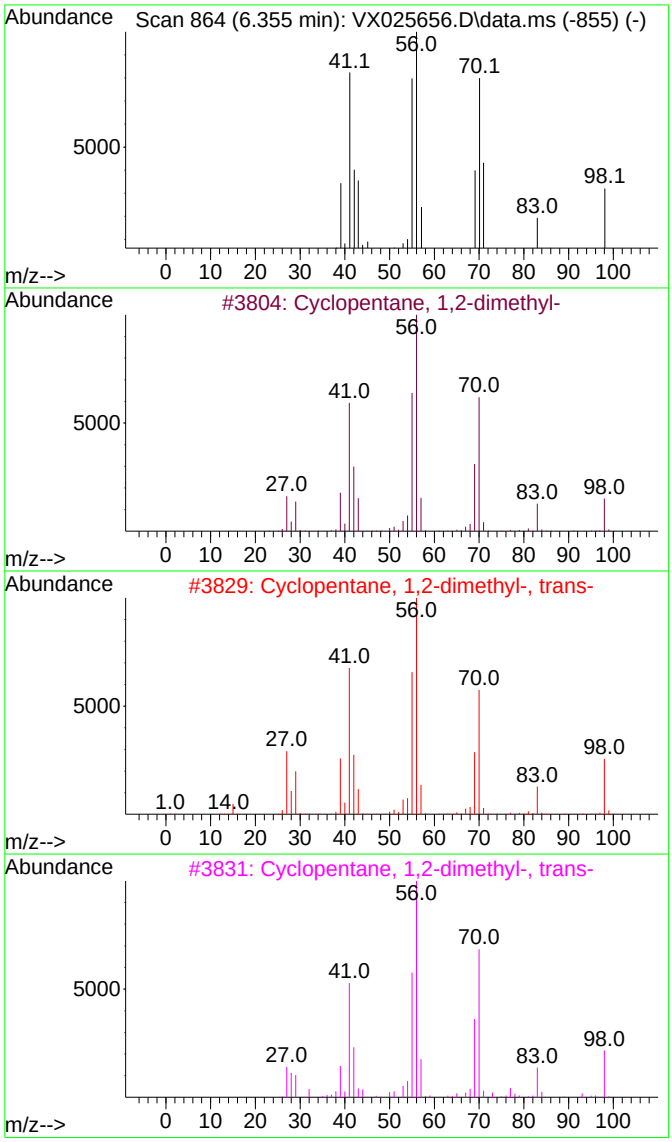
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

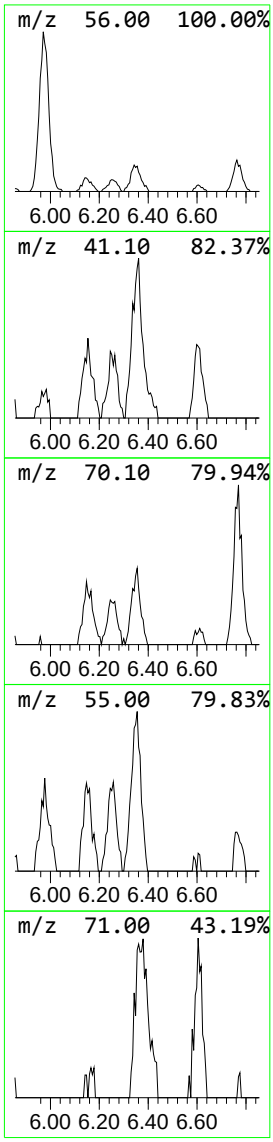
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Cyclic6.355 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.355	3.03 ug/L	19138	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	87
2	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	87
3	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	81
4	1-Heptene	98	C7H14	000592-76-7	81
5	1-Heptene	98	C7H14	000592-76-7	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

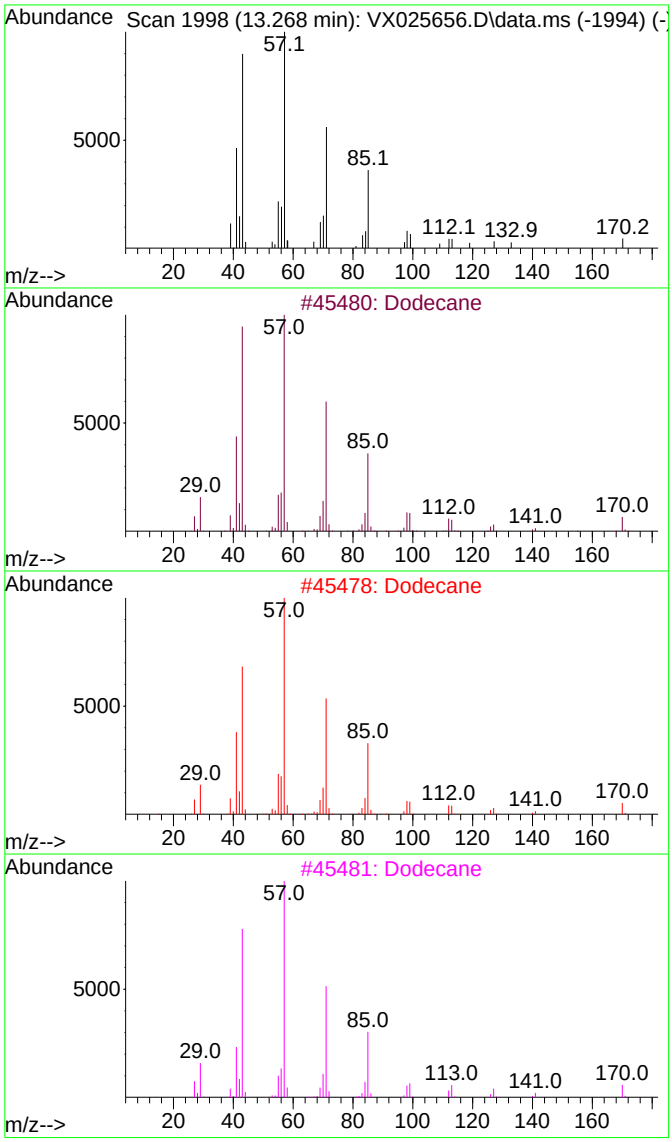
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

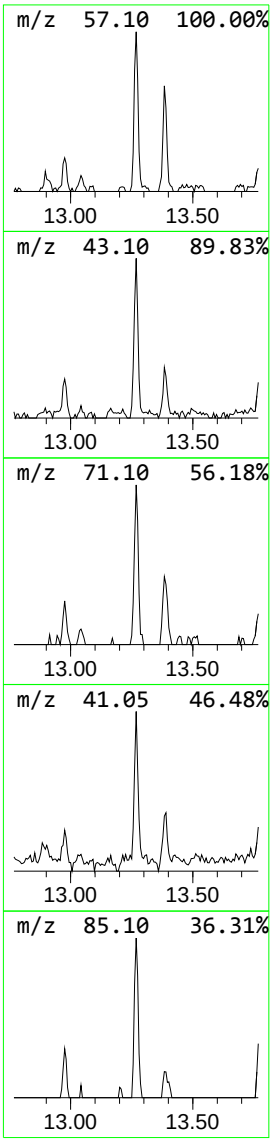
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.268	2.54 ug/L	19806	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	95
2	Dodecane	170	C12H26	000112-40-3	94
3	Dodecane	170	C12H26	000112-40-3	93
4	Dodecane	170	C12H26	000112-40-3	91
5	Undecane	156	C11H24	001120-21-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

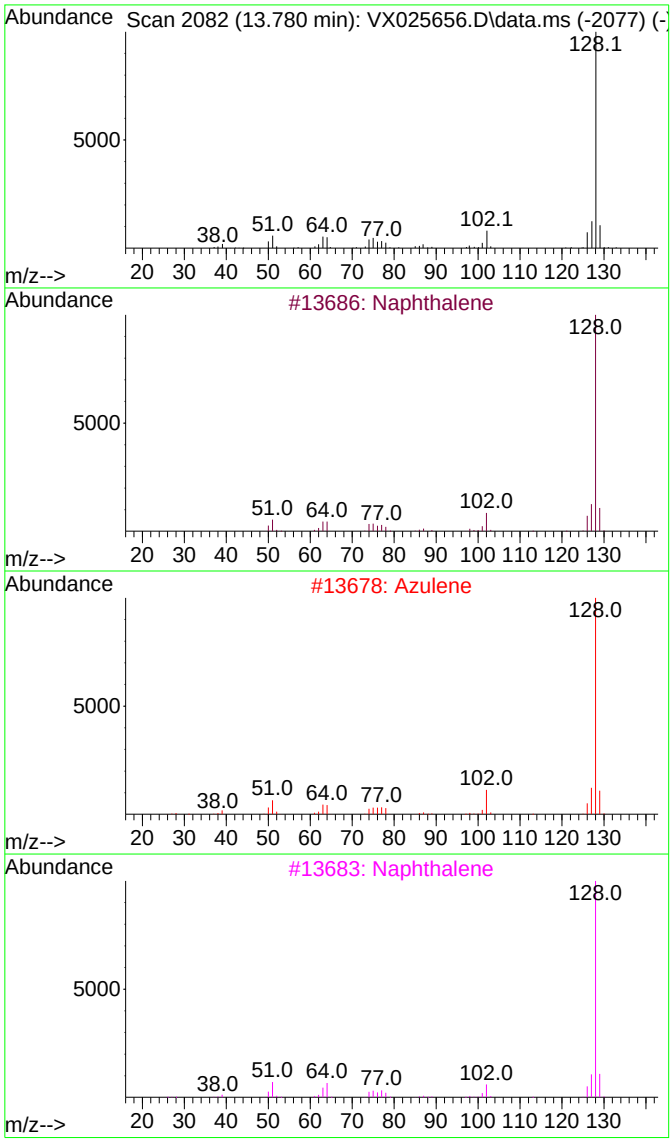
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

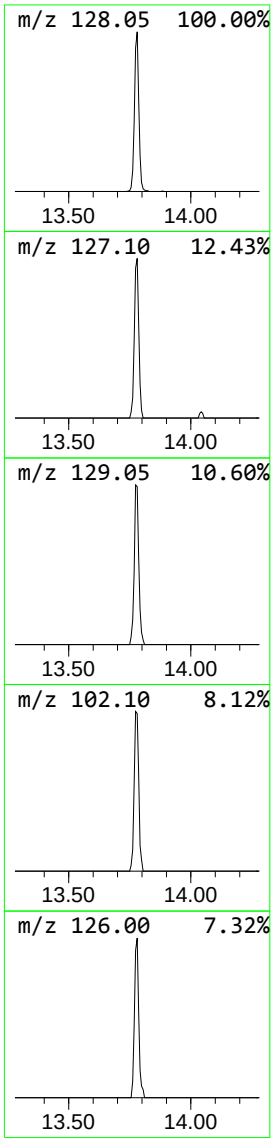
****

Peak Number 5 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	6.43 ug/L	50061	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	93
3	Naphthalene	128	C10H8	000091-20-3	93
4	Azulene	128	C10H8	000275-51-4	91
5	Azulene	128	C10H8	000275-51-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

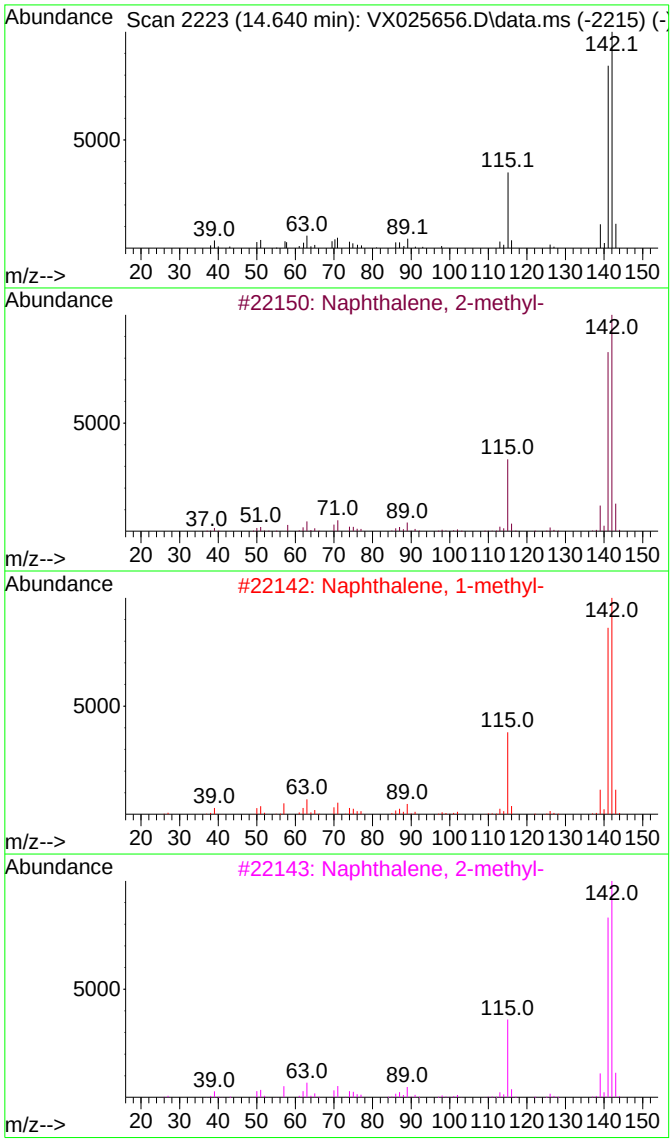
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

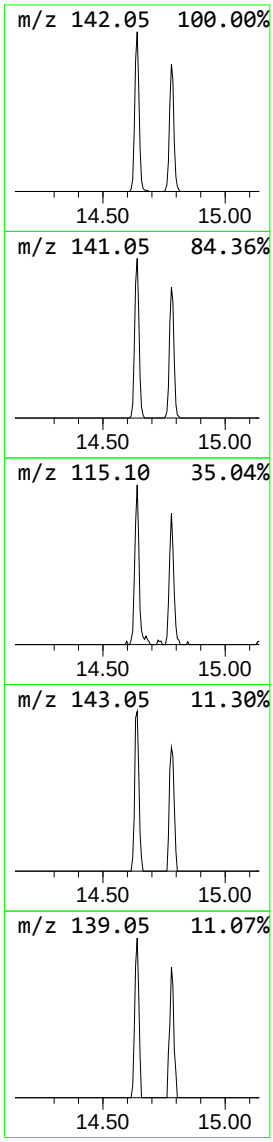
****

Peak Number 6 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	4.83 ug/L	37624	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
4	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

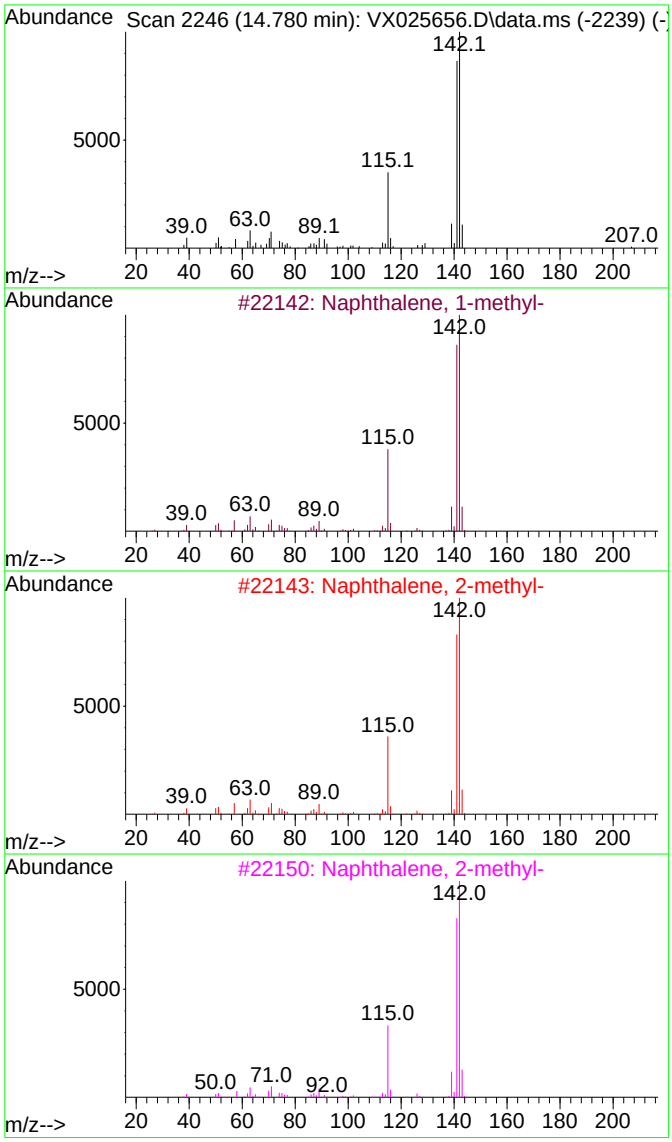
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

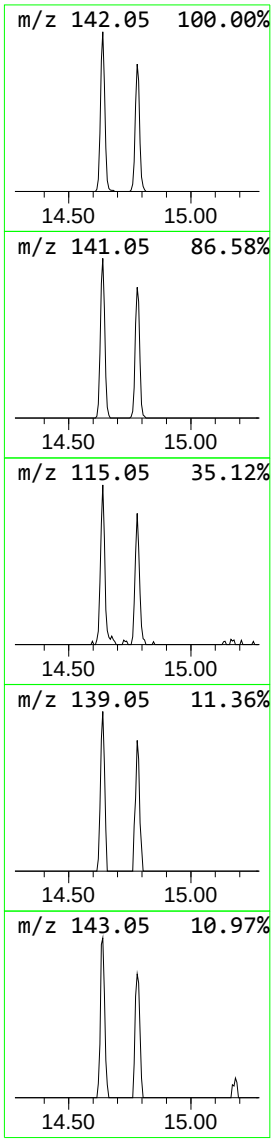
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	4.85 ug/L	37781	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
Data File : VX025656.D
Acq On : 09 Dec 2021 13:31
Operator : JC/MD
Sample : M4884-20ME
Misc : 4.95g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9K4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: C...	4.288	3.1	ug/L	19861	1	6.769	315345	50.0
(DEL) Alkane: C...	6.355	3.0	ug/L	19138	1	6.769	315345	50.0
(DEL) Alkane: S...	13.268	2.5	ug/L	19806	3	12.024	389504	50.0
Azulene	13.780	6.4	ug/L	50061	3	12.024	389504	50.0
Naphthalene, 2-...	14.640	4.8	ug/L	37624	3	12.024	389504	50.0
Naphthalene, 1-...	14.780	4.8	ug/L	37781	3	12.024	389504	50.0