LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX060922\
Data File : VX029345.D
Acq On : 09 Jun 2022 15:11
Operator : JC/MD
Sample : N3209-04
Misc : 5.20g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14B-4-GR

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\82X060722W.M
Title : SW846 8260

Signal : TIC: VX029345.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.550	721	732	737	rVV	267361	784079	7.96%	0.305%
2	5.611	737	742	760	rVB2	277157	822196	8.35%	0.320%
3	6.763	920	931	942	rBV	388239	916626	9.31%	0.357%
4	7.360	1019	1029	1042	rVB	614981	1474845	14.98%	0.574%
5	7.775	1087	1097	1106	rVB2	963154	2002513	20.33%	0.780%
6	8.604	1225	1233	1234	rBV2	821758	1292660	13.13%	0.503%
7	8.641	1234	1239	1251	rVB2	1628966	3819008	38.78%	1.487%
8	8.775	1254	1261	1265	rVV	1095183	1790716	18.18%	0.697%
9	8.976	1289	1294	1301	rVB2	2291515	3808095	38.67%	1.483%
10	9.104	1306	1315	1320	rBV	825788	1393144	14.15%	0.543%
11	9.506	1375	1381	1387	rBV3	1473448	3051814	30.99%	1.189%
12	9.622	1394	1400	1404	rBV	3574054	5863354	59.54%	2.284%
13	9.762	1416	1423	1428	rBV2	819988	1345658	13.66%	0.524%
14	9.829	1428	1434	1438	rBV2	1909521	3719227	37.77%	1.449%
15	9.866	1438	1440	1447	rVB2	645789	929812	9.44%	0.362%
16	10.000	1456	1462	1467	rVB2	552614	958082	9.73%	0.373%
17	10.055	1467	1471	1476	rBV	864733	1181930	12.00%	0.460%
18	10.128	1476	1483	1487	rBV2	710328	1434762	14.57%	0.559%
19	10.183	1487	1492	1499	rVB2	813355	1370552	13.92%	0.534%
20	10.275	1499	1507	1511	rBV2	1640804	3349666	34.01%	1.305%
21	10.317	1511	1514	1518	rVV	1998367	2885572	29.30%	1.124%
22	10.354	1518	1520	1532	rVB	1454352	2567596	26.07%	1.000%
23	10.457	1532	1537	1546	rBV2	1058165	1651383	16.77%	0.643%
24	10.585	1551	1558	1566	rBV3	2677243	5233397	53.14%	2.038%
25	10.671	1566	1572	1577	rBV4	777247	1628945	16.54%	0.634%
26	10.781	1582	1590	1594	rBV2	3219566	5666350	57.54%	2.207%
27	10.860	1594	1603	1606	rBV3	4057829	6616759	67.19%	2.577%
28	10.896	1606	1609	1614	rVB	2130053	2923612	29.69%	1.139%
29	10.951	1614	1618	1623	rBV3	625573	1052833	10.69%	0.410%
30	11.006	1623	1627	1629	rBV2	889656	1342405	13.63%	0.523%
31	11.030	1629	1631	1636	rVB2	1139077	1338678	13.59%	0.521%
32	11.085	1636	1640	1644	rVB2	961248	1295288	13.15%	0.504%
33	11.128	1644	1647	1651	rVB	867755	1016331	10.32%	0.396%
34	11.219	1655	1662	1671	rVB3	3296362	5574069	56.60%	2.171%
35	11.341	1673	1682	1686	rBV4	1065533	2399893	24.37%	0.935%
36	11.390	1686	1690	1694	rBV3	1067077	1449229	14.72%	0.564%

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ClientSampleId :
WC-14B-4-GR

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Title : SW846 8260

37	11.433	1694	1697	1701	rVB	2220895	2634995	26.76%	1.026%
38	11.482	1701	1705	1709	rVB3	1299155	2022076	20.53%	0.788%
39	11.634	1723	1730	1734	rVB6	1004839	2529324	25.68%	0.985%
40	11.719	1741	1744	1746	rBV2	717096	811640	8.24%	0.316%
41	11.866	1759	1768	1770	rBV2	1291267	2730517	27.73%	1.063%
42	11.890	1770	1772	1777	rVV	2171558	3304230	33.55%	1.287%
43	11.945	1777	1781	1784	rVV	2454794	3315184	33.66%	1.291%
44	11.975	1784	1786	1790	rVV3	720155	940184	9.55%	0.366%
45	12.030	1791	1795	1800	rVB2	1056934	1649998	16.75%	0.643%
46	12.158	1812	1816	1819	rBV5	552200	762266	7.74%	0.297%
47	12.250	1826	1831	1835	rBV	2236531	2972669	30.19%	1.158%
48	12.311	1837	1841	1849	rVV2	2584295	5422046	55.06%	2.112%
49	12.408	1853	1857	1864	rVV2	1435817	3624905	36.81%	1.412%
50	12.469	1864	1867	1872	rVV4	1360846	2340631	23.77%	0.912%
51	12.561	1876	1882	1886	rVV5	924271	2091911	21.24%	0.815%
52	12.616	1887	1891	1895	rVV	4582179	6106794	62.01%	2.378%
53	12.646	1895	1896	1900	rVV2	875492	853481	8.67%	0.332%
54	12.707	1900	1906	1913	rVV5	2413790	5306919	53.89%	2.067%
55	12.762	1913	1915	1920	rVB5	691798	904506	9.18%	0.352%
56	12.823	1920	1925	1931	rVB3	2130169	3792058	38.51%	1.477%
57	12.896	1931	1937	1939	rBV3	1771275	3174917	32.24%	1.237%
58	12.926	1939	1942	1946	rVB	3616306	4405849	44.74%	1.716%
59	12.987	1947	1952	1955	rBV2	1940408	2381018	24.18%	0.927%
60	13.024	1955	1958	1965	rVB2	1585584	2482813	25.21%	0.967%
61	13.097	1966	1970	1974	rBV	1423727	1863085	18.92%	0.726%
62	13.140	1974	1977	1980	rBV2	1521757	1870105	18.99%	0.728%
63	13.292	1998	2002	2008	rVB2	5281487	7991243	81.15%	3.112%
64	13.372	2012	2015	2018	rVV	1424894	1436488	14.59%	0.559%
65	13.420	2018	2023	2033	rVB10	1252247	3488340	35.42%	1.359%
66	13.506	2033	2037	2040	rBV2	1130023	1581081	16.05%	0.616%
67	13.542	2040	2043	2046	rVB	1162149	1369529	13.91%	0.533%
68	13.585	2046	2050	2054	rBV3	2916162	3635263	36.91%	1.416%
69	13.640	2054	2059	2061	rVV4	1186415	2322939	23.59%	0.905%
70	13.670	2061	2064	2069	rVV2	2426546	3916400	39.77%	1.525%
71	13.756	2072	2078	2081	rBV2	1693552	2531441	25.71%	0.986%
72	13.798	2081	2085	2089	rBV2	1555636	2044162	20.76%	0.796%
73	13.853	2091	2094	2099	rVB3	993288	1460444	14.83%	0.569%
74	13.926	2099	2106	2111	rBV5	2042892	4292890	43.59%	1.672%
75	13.975	2111	2114	2117	rBV3	982703	1494189	15.17%	0.582%
76	14.073	2125	2130	2133	rBV2	1353522	1885809	19.15%	0.734%

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ClientSampleId :
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Integration Parameters: RTEINT.P
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Title : SW846 8260

77	14.164	2139	2145	2149	rVV2	862527	1208613	12.27%	0.471%
78	14.219	2149	2154	2162	rVV3	3082908	5703091	57.91%	2.221%
79	14.323	2168	2171	2176	rVV	1803531	2508560	25.47%	0.977%
80	14.377	2176	2180	2184	rVV2	1850387	2295651	23.31%	0.894%
81	14.420	2184	2187	2193	rVB4	1212967	1717568	17.44%	0.669%
82	14.487	2193	2198	2206	rBV3	2434705	4576089	46.47%	1.782%
83	14.579	2210	2213	2216	rVV3	552291	748727	7.60%	0.292%
84	14.615	2216	2219	2225	rVV5	1272250	1847648	18.76%	0.720%
85	14.676	2225	2229	2233	rVB	1761089	2235644	22.70%	0.871%
86	14.725	2233	2237	2241	rBV2	1080008	1702928	17.29%	0.663%
87	14.792	2244	2248	2251	rBV3	937212	1383676	14.05%	0.539%
88	14.853	2255	2258	2261	rVB2	769623	835358	8.48%	0.325%
89	14.981	2276	2279	2283	rVB	599546	827679	8.40%	0.322%
90	15.048	2286	2290	2293	rBV3	567800	861565	8.75%	0.336%
91	15.188	2307	2313	2319	rVB3	1171520	2236196	22.71%	0.871%
92	15.261	2319	2325	2331	rVB6	511838	1141092	11.59%	0.444%
93	15.383	2341	2345	2347	rBV2	604484	872908	8.86%	0.340%
94	15.408	2347	2349	2353	rVB	1157292	1459738	14.82%	0.569%
95	15.487	2357	2362	2366	rVB	3054715	4271592	43.38%	1.664%
96	15.615	2378	2383	2387	rBV	6228011	9847981	100.00%	3.835%
97	15.652	2387	2389	2397	rVB	3103350	4497193	45.67%	1.752%
98	15.737	2397	2403	2408	rBV2	679875	1247554	12.67%	0.486%
99	15.841	2411	2420	2430	rVB	1835033	5248517	53.30%	2.044%
100	15.993	2439	2445	2456	rVB	922563	1788266	18.16%	0.696%

Sum of corrected areas: 256759252

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Instrument :
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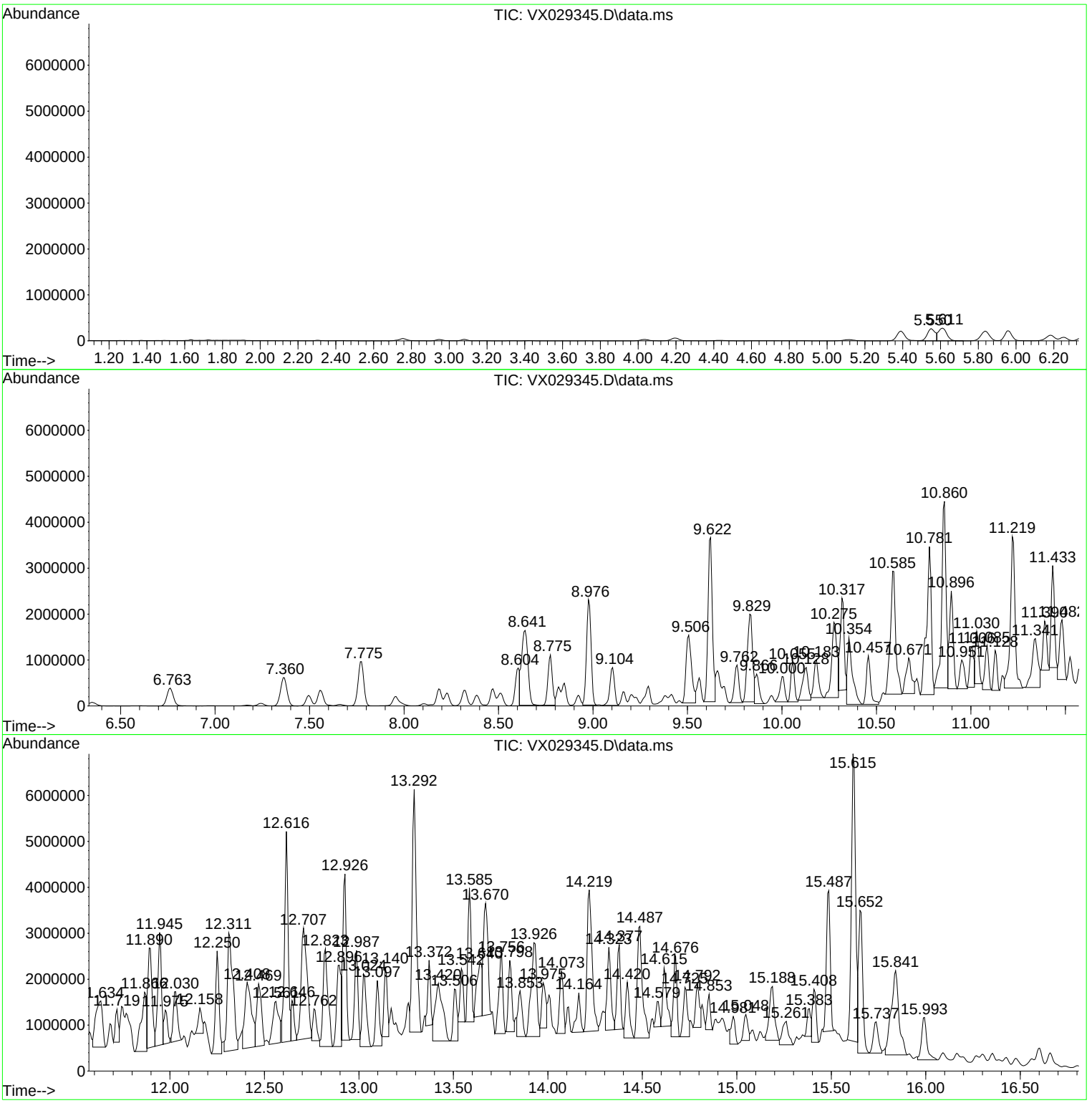
ClientSampleId :
WC-14B-4-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.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 :
WC-14B-4-GR

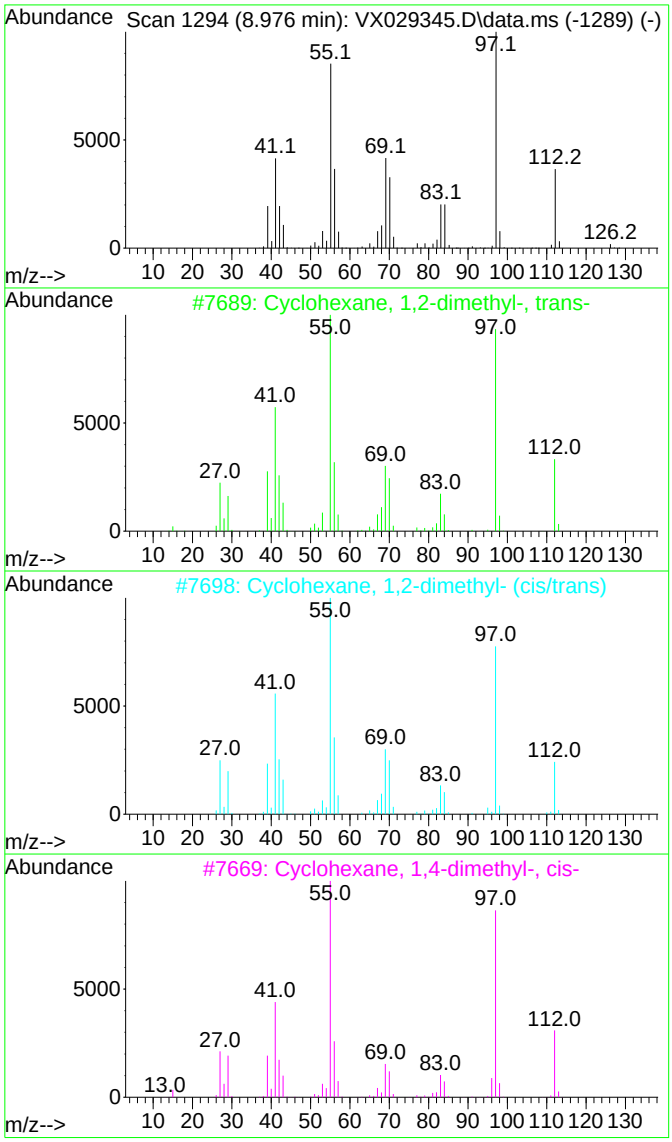
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

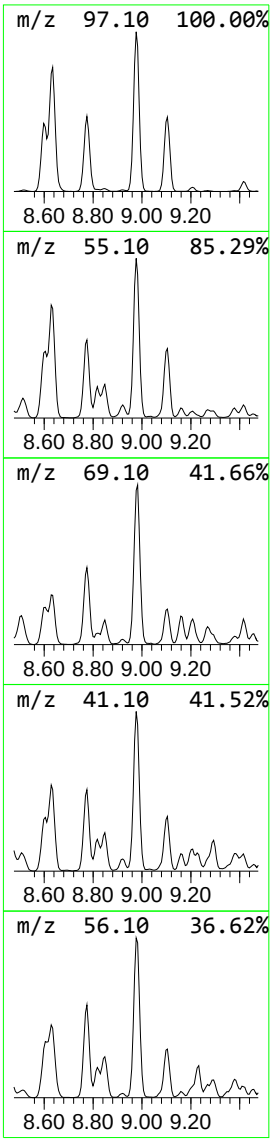
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclohexane, 1,2-dimethyl-,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.976	161.10 ug/l	3808100	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	94
2	Cyclohexane, 1,2-dimethyl- (cis/...	112	C8H16	000583-57-3	90
3	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	72
4	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	72
5	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	72





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Instrument :
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ClientSampleId :
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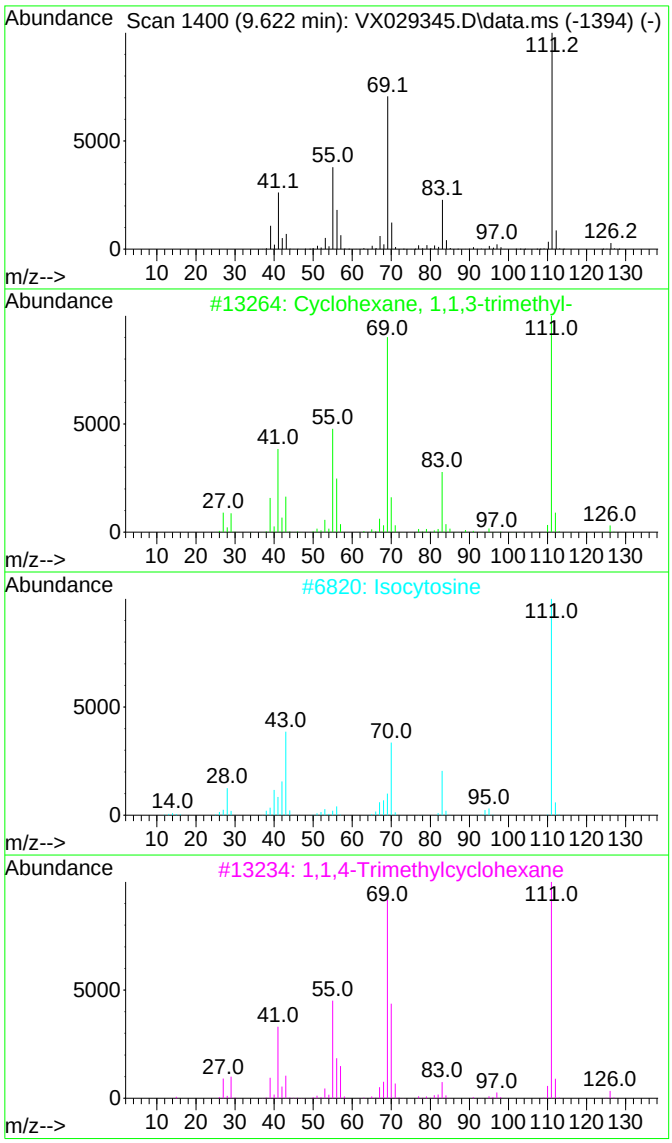
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

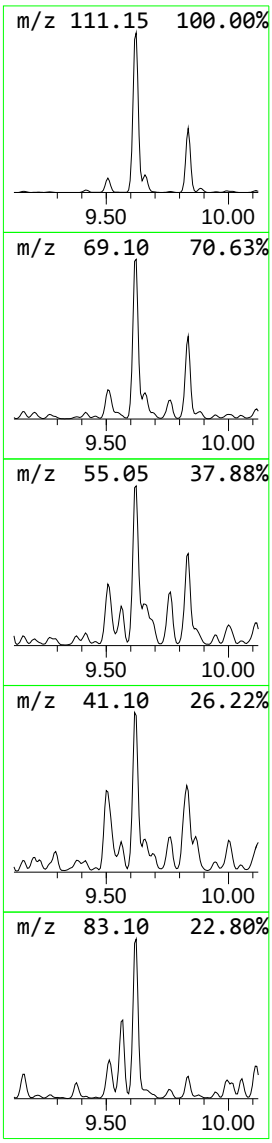
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.622	248.04 ug/l	5863350	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	95
2	Isocytosine	111	C4H5N3O	000108-53-2	72
3	1,1,4-Trimethylcyclohexane	126	C9H18	007094-27-1	64
4	1-Aminocyclopropanecarboxylic ac...	156	C7H12N2O2	1000375-50-8	59
5	4-Amino-6-hydroxypyrimidine	111	C4H5N3O	001193-22-2	50





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Instrument :
MSVOA_X
ClientSampleId :
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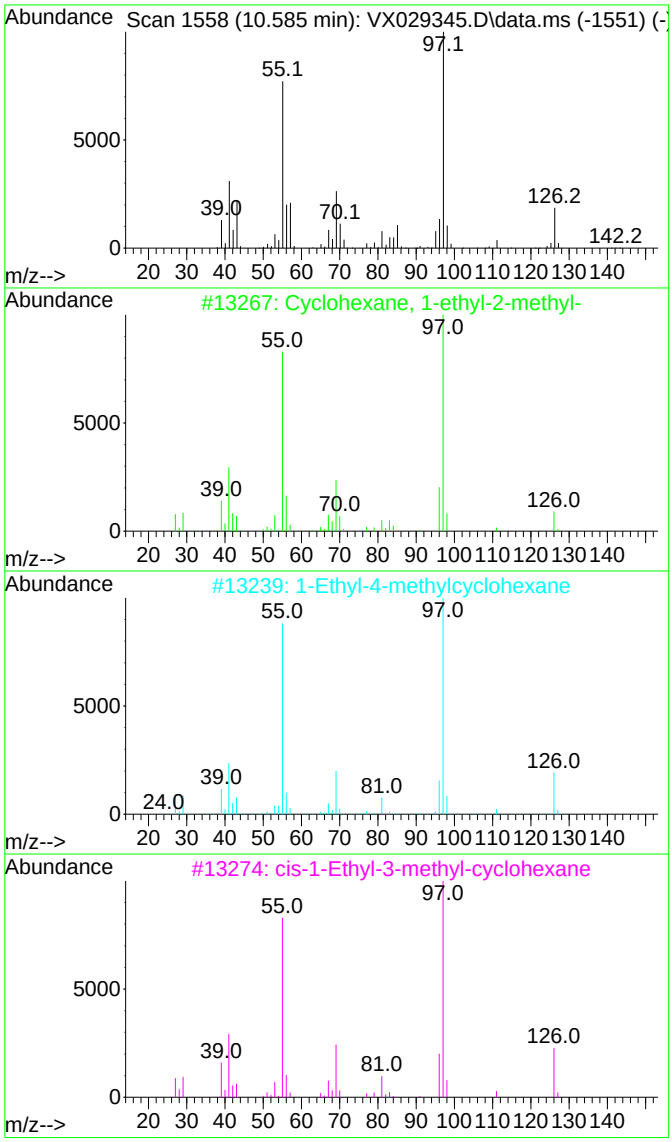
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

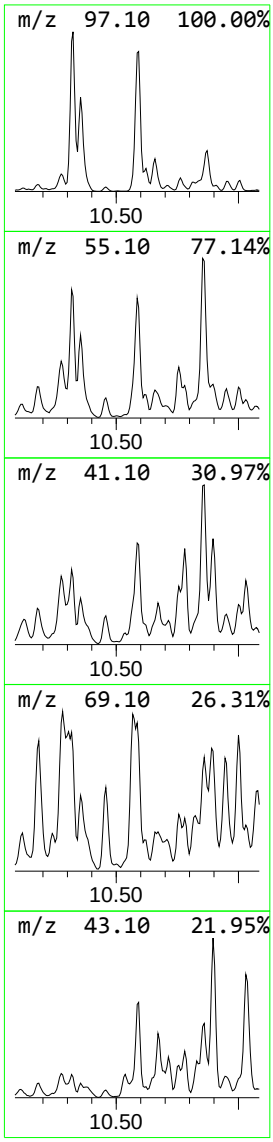
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.585	221.39 ug/l	5233400	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	87
2	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	81
3	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	81
4	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	76
5	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	76





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14B-4-GR

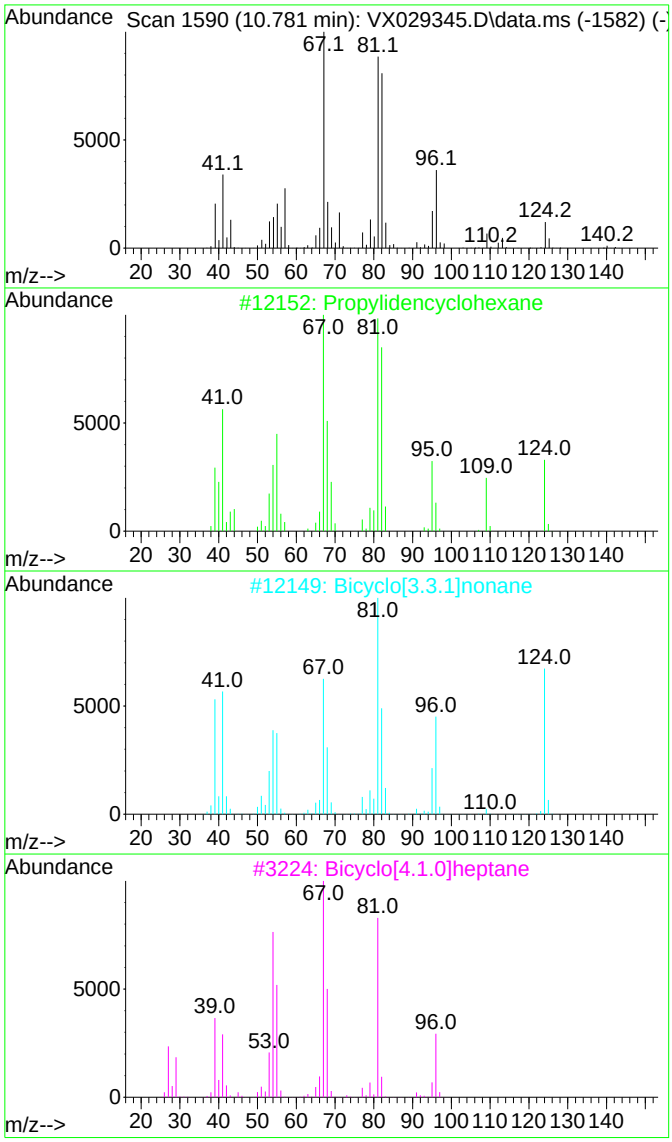
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

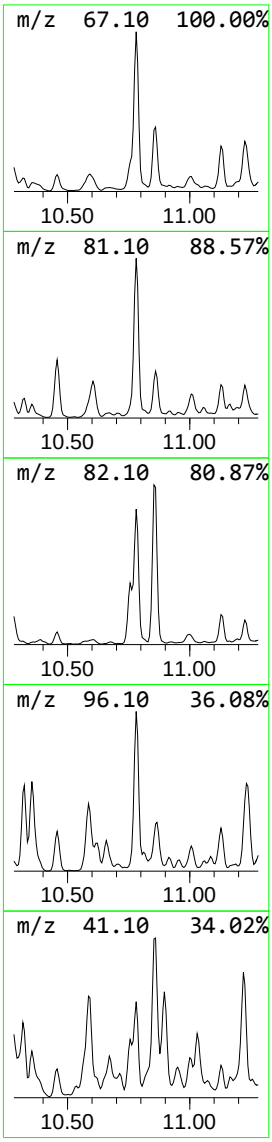
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propylidencyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.781	239.71 ug/l	5666350	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylidencyclohexane	124	C9H16	002129-93-3	80
2	Bicyclo[3.3.1]nonane	124	C9H16	000280-65-9	60
3	Bicyclo[4.1.0]heptane	96	C7H12	000286-08-8	52
4	1H-Indene, octahydro-, trans-	124	C9H16	003296-50-2	49
5	2-Cyclohexen-1-one, 4,5-dimethyl-	124	C8H12O	005715-25-3	43





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Instrument :
MSVOA_X
ClientSampleId :
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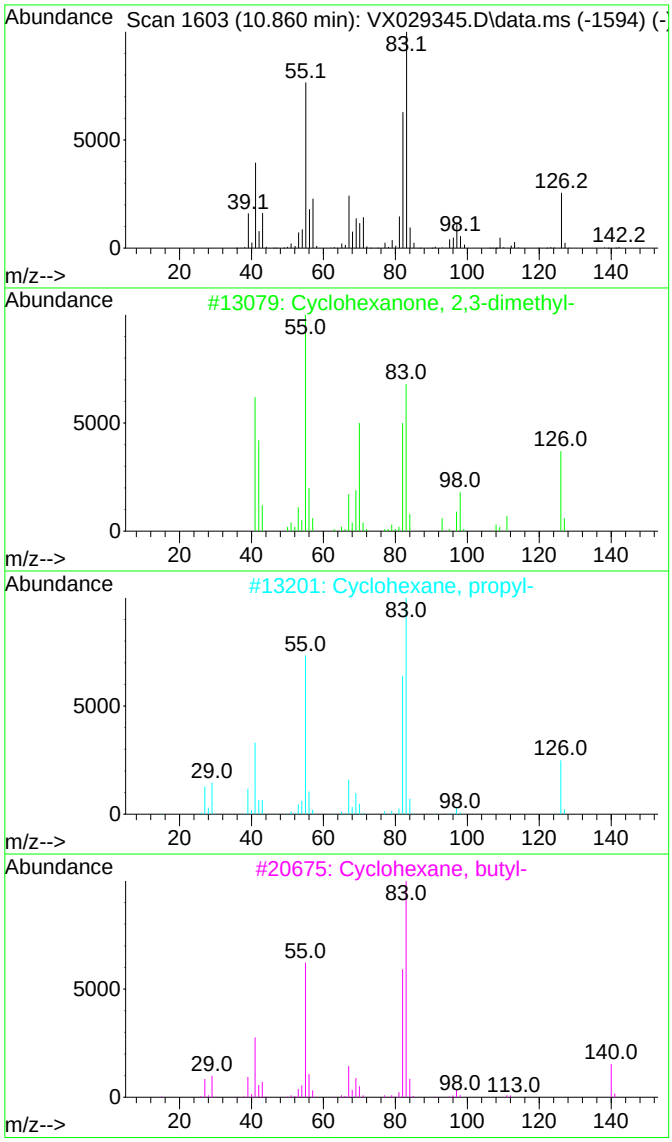
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

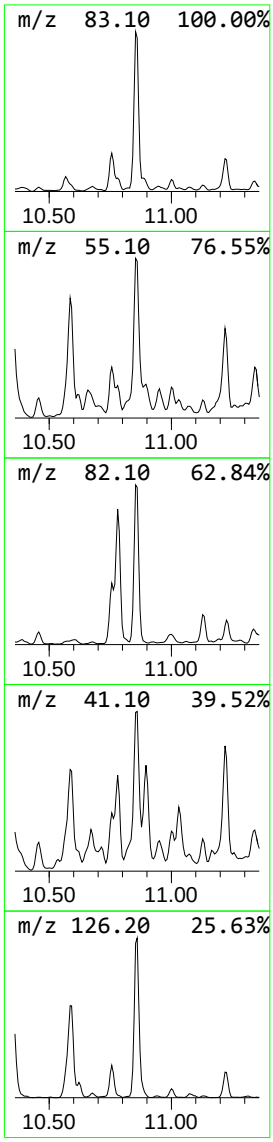
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclohexanone, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.860	279.91 ug/l	6616760	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2,3-dimethyl-	126	C8H14O	013395-76-1	87
2	Cyclohexane, propyl-	126	C9H18	001678-92-8	87
3	Cyclohexane, butyl-	140	C10H20	001678-93-9	64
4	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	62
5	Cyclohexane, (3-methylpentyl)-	168	C12H24	061142-38-9	59





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Data File : VX029345.D
Acq On : 09 Jun 2022 15:11
Operator : JC/MD
Sample : N3209-04
Misc : 5.20g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14B-4-GR

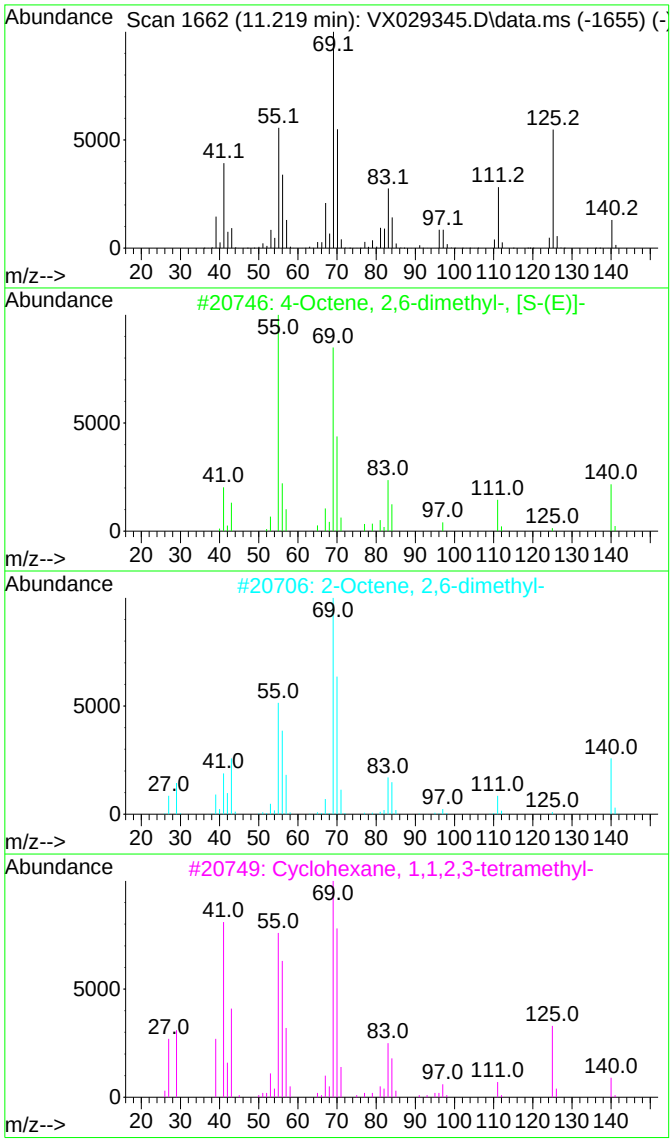
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

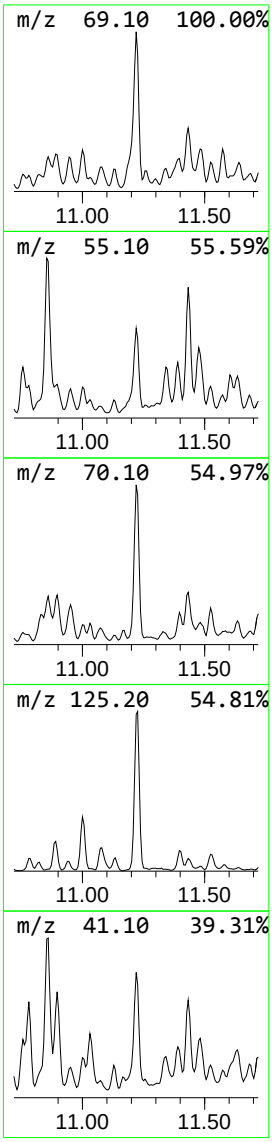
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4-Octene, 2,6-dimethyl-, [S... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.220	168.91 ug/l	5574070	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	62
2	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	58
3	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	53
4	(1,2,4-Trimethylcyclohexyl)metha...	198	C12H22O2	1010499-04-6	47
5	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	47





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Data File : VX029345.D
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Operator : JC/MD
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Misc : 5.20g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14B-4-GR

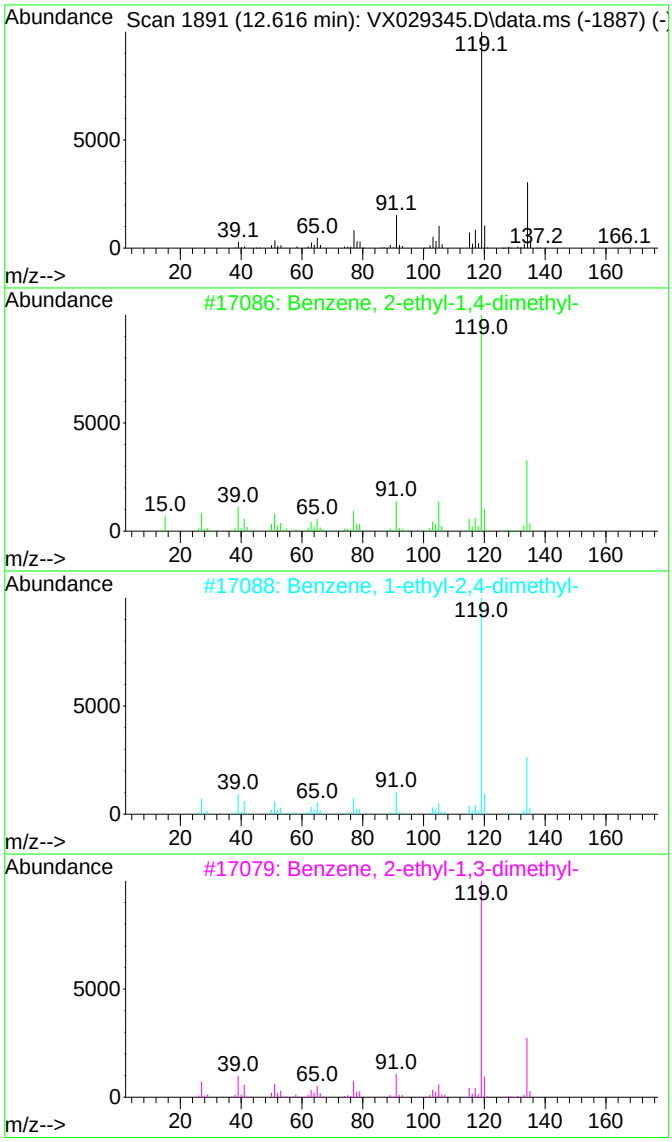
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

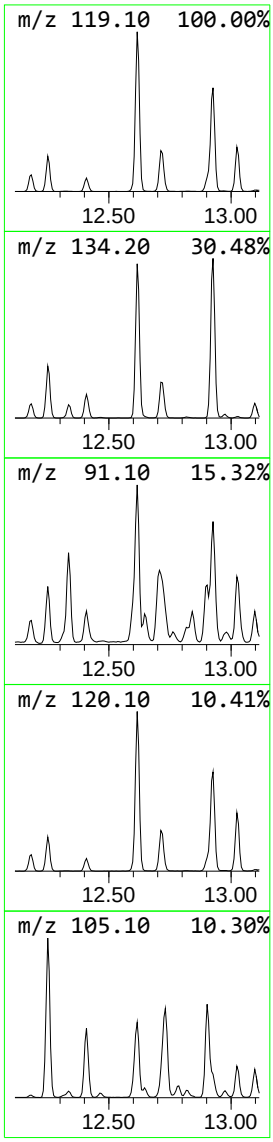
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	185.06 ug/l	6106790	1,4-Dichlorobenzene-d4	12.024

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-2,4-dimethyl-	134	C10H14	000874-41-9	95
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95





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Data File : VX029345.D
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Operator : JC/MD
Sample : N3209-04
Misc : 5.20g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14B-4-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

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

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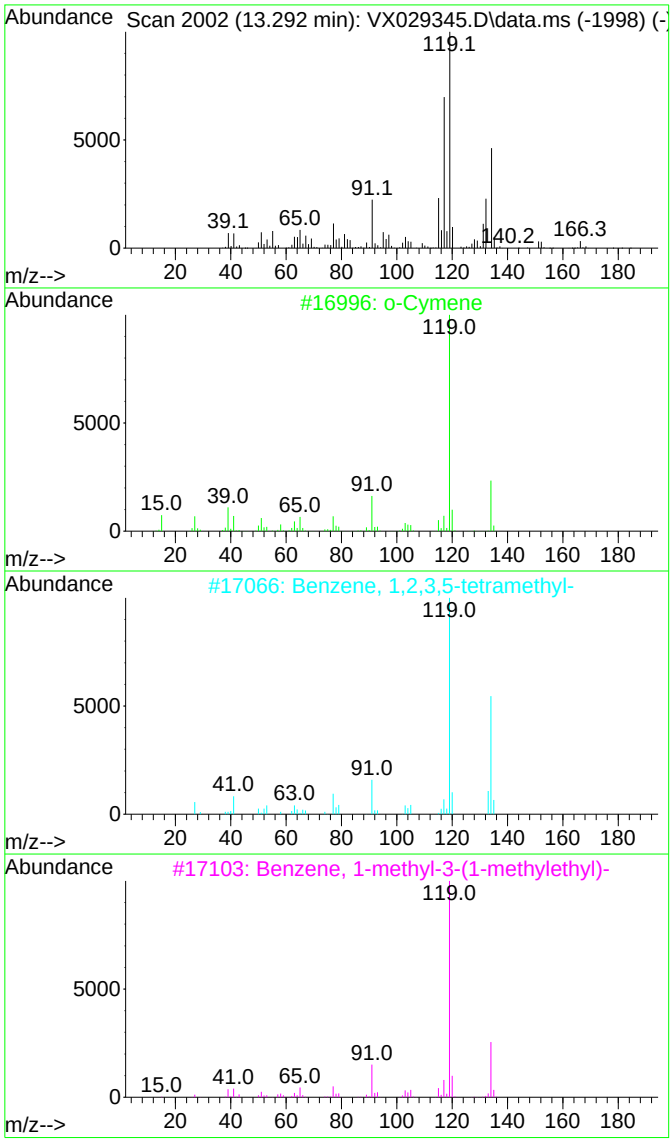
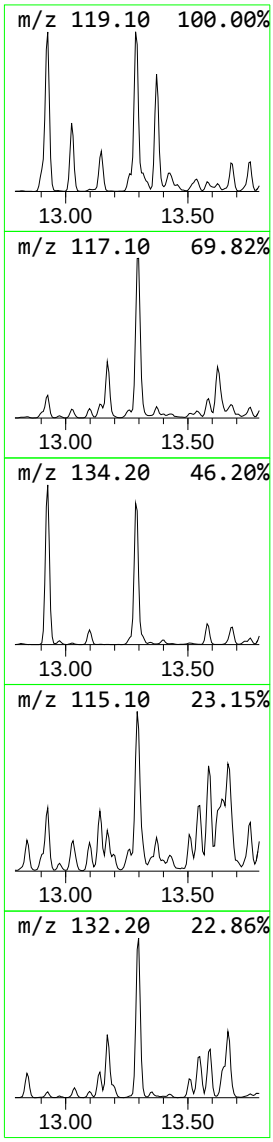
Peak Number 8 o-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	242.16 ug/l	7991240	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	60
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	60
3	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	60
4	p-Cymene	134	C10H14	000099-87-6	60
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	60





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Operator : JC/MD
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Misc : 5.20g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14B-4-GR

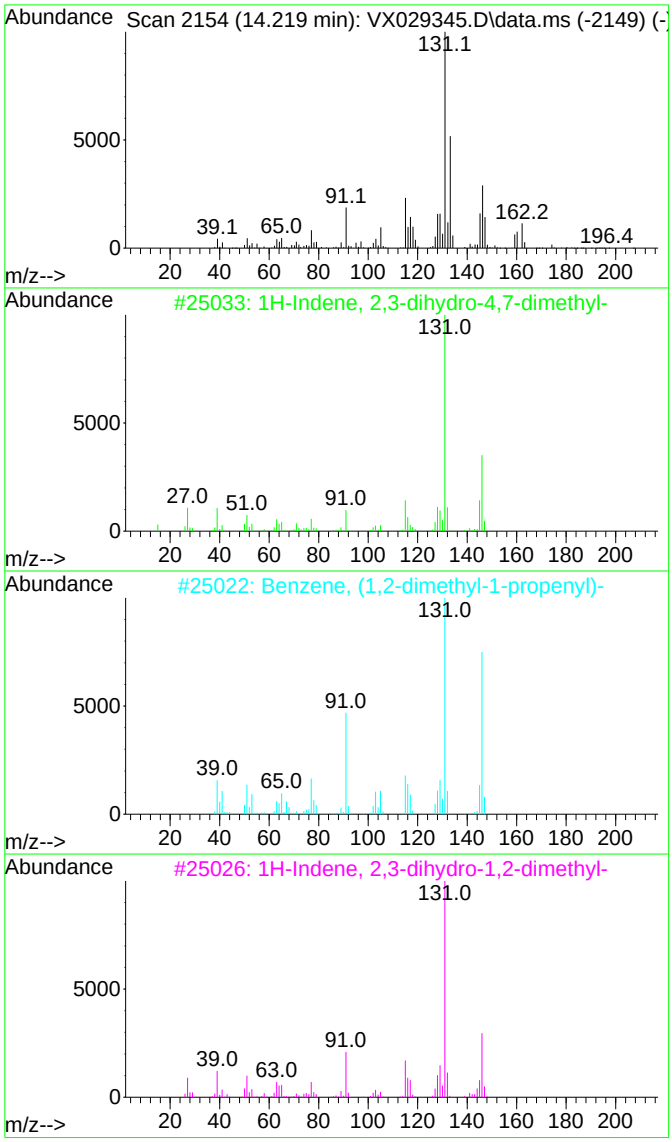
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

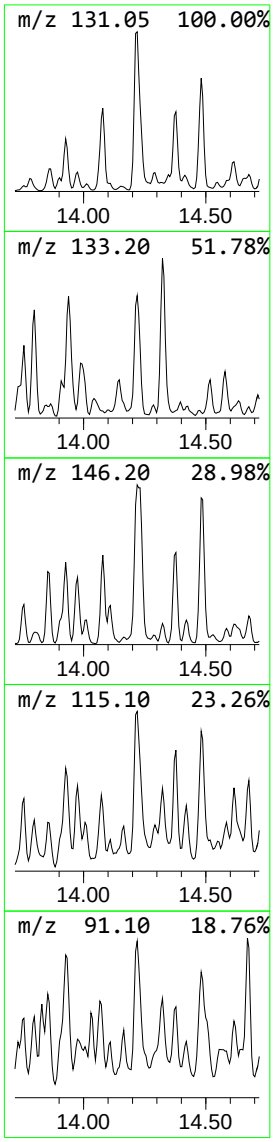
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.219	172.82 ug/l	5703090	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
2	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	64
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	62
4	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	60
5	1H-Indene, 2,3-dihydro-4,6-dimet...	146	C11H14	001685-82-1	60





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Operator : JC/MD
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Misc : 5.20g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-14B-4-GR

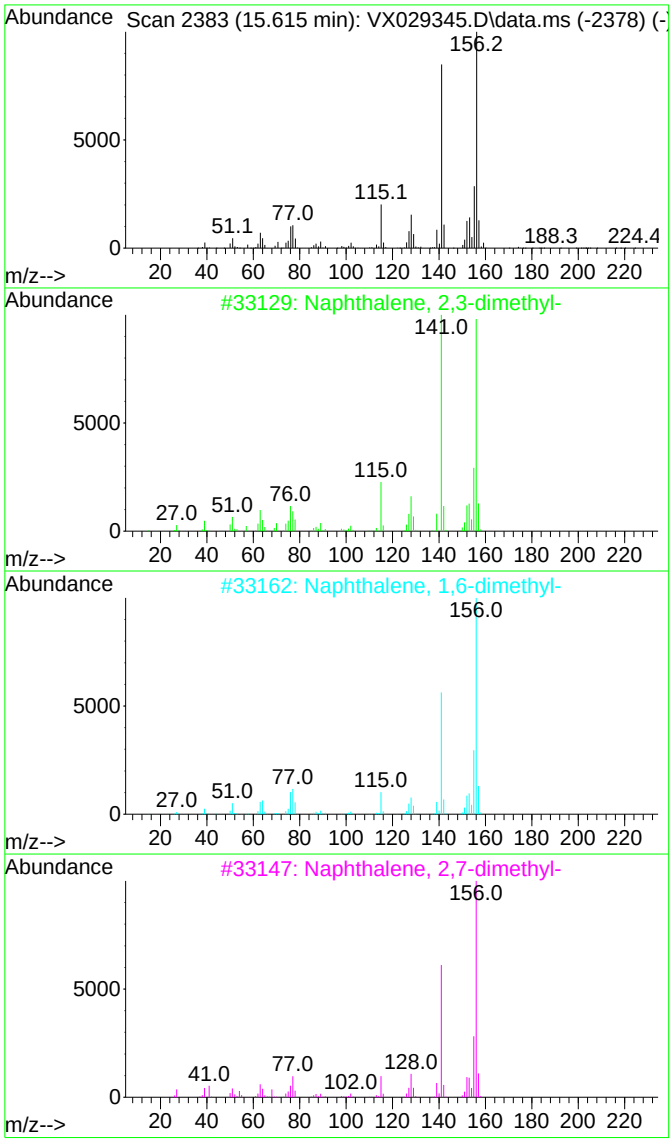
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X060722W.M
Quant Title : SW846 8260

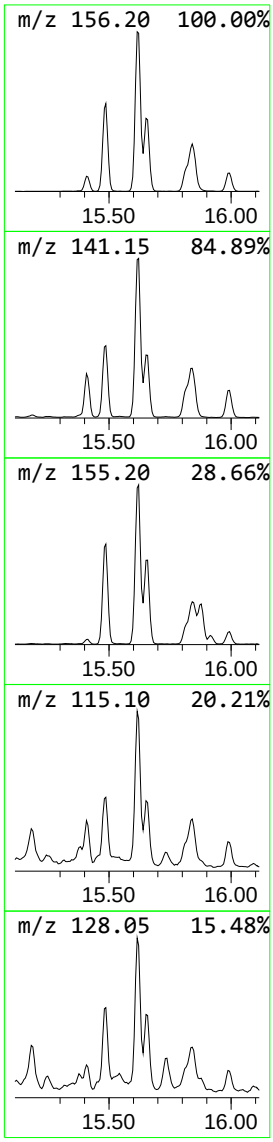
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	298.42 ug/l	9847980	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	96
5	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96





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
Cyclohexane, 1,...	8.976	161.1	ug/l	3808100	3	10.055	1181930	50.0
Cyclohexane, 1,...	9.622	248.0	ug/l	5863350	3	10.055	1181930	50.0
Cyclohexane, 1-...	10.585	221.4	ug/l	5233400	3	10.055	1181930	50.0
Propylidencyclo...	10.781	239.7	ug/l	5666350	3	10.055	1181930	50.0
Cyclohexanone, ...	10.860	279.9	ug/l	6616760	3	10.055	1181930	50.0
4-Octene, 2,6-d...	11.220	168.9	ug/l	5574070	4	12.024	1650000	50.0
Benzene, 2-ethy...	12.616	185.1	ug/l	6106790	4	12.024	1650000	50.0
o-Cymene	13.292	242.2	ug/l	7991240	4	12.024	1650000	50.0
1H-Indene, 2,3-...	14.219	172.8	ug/l	5703090	4	12.024	1650000	50.0
Naphthalene, 2,...	15.615	298.4	ug/l	9847980	4	12.024	1650000	50.0