LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041122\
Data File : VN071931.D
Acq On : 11 Apr 2022 13:16
Operator : JC\MD
Sample : N2306-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

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_N\methods\82N033022W.M
Title : SW846 8260

Signal : TIC: VN071931.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	33	41	62	rBV2	132220	431969	4.28%	0.282%
2	8.010	1014	1024	1029	rBV	370394	909840	9.02%	0.594%
3	8.075	1029	1035	1045	rVV	742494	1759402	17.45%	1.149%
4	8.281	1062	1070	1085	rVB	90420	211651	2.10%	0.138%
5	8.428	1085	1095	1107	rBV	396235	899257	8.92%	0.587%
6	8.816	1154	1161	1176	rVB2	113355	235804	2.34%	0.154%
7	8.957	1176	1185	1200	rBV	1084080	2253260	22.34%	1.471%
8	9.451	1255	1269	1275	rBV2	54828	133596	1.32%	0.087%
9	10.433	1428	1436	1442	rBV	1756456	3315920	32.88%	2.165%
10	10.498	1442	1447	1460	rVV	2082927	3972256	39.39%	2.594%
11	10.616	1460	1467	1474	rVB	161440	298653	2.96%	0.195%
12	11.045	1531	1540	1545	rBV	57451	102082	1.01%	0.067%
13	11.286	1573	1581	1585	rVV	108719	220294	2.18%	0.144%
14	11.339	1585	1590	1596	rVB	105727	203132	2.01%	0.133%
15	11.445	1603	1608	1613	rBV3	91151	159768	1.58%	0.104%
16	11.522	1613	1621	1633	rVB3	339075	854817	8.48%	0.558%
17	11.622	1633	1638	1643	rBV	333830	520837	5.16%	0.340%
18	11.739	1651	1658	1669	rBV	1592951	2885655	28.62%	1.884%
19	11.839	1669	1675	1679	rBV	370278	635514	6.30%	0.415%
20	11.951	1684	1694	1703	rBV3	2777717	5501433	54.56%	3.592%
21	12.027	1703	1707	1712	rVB3	265897	460761	4.57%	0.301%
22	12.086	1712	1717	1724	rBV5	43614	106686	1.06%	0.070%
23	12.169	1724	1731	1737	rVB4	98299	186313	1.85%	0.122%
24	12.251	1737	1745	1746	rBV3	540798	976635	9.68%	0.638%
25	12.274	1746	1749	1757	rVB	672119	1143509	11.34%	0.747%
26	12.363	1759	1764	1768	rVB	524060	766229	7.60%	0.500%
27	12.410	1768	1772	1774	rBV3	97506	144448	1.43%	0.094%
28	12.486	1774	1785	1795	rBV7	635526	2071407	20.54%	1.352%
29	12.569	1795	1799	1803	rBV2	191443	384472	3.81%	0.251%
30	12.621	1803	1808	1809	rBV4	212281	296696	2.94%	0.194%
31	12.651	1810	1813	1816	rBV	318052	408912	4.06%	0.267%
32	12.727	1821	1826	1830	rVV	1437582	2405386	23.85%	1.571%
33	12.763	1830	1832	1836	rVV	545168	616123	6.11%	0.402%
34	12.816	1837	1841	1844	rVV4	158675	215975	2.14%	0.141%
35	12.910	1850	1857	1862	rVB3	494902	1123986	11.15%	0.734%
36	12.974	1862	1868	1872	rBV2	1494976	2742692	27.20%	1.791%

LSC Area Percent Report

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Sample : N2306-01
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Instrument :
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ClientSampleId :
2404-2405

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_N\methods\82N033022W.M
Title : SW846 8260

37	13.045	1872	1880	1886	rVV2	5092245	10084077	100.00%	6.584%
38	13.104	1886	1890	1895	rVB	730489	1145312	11.36%	0.748%
39	13.216	1895	1909	1916	rBV4	814551	3069388	30.44%	2.004%
40	13.280	1916	1920	1927	rVB3	1017855	1804092	17.89%	1.178%
41	13.363	1927	1934	1939	rBV	2765897	4617674	45.79%	3.015%
42	13.492	1952	1956	1960	rVB3	520576	770436	7.64%	0.503%
43	13.557	1960	1967	1971	rBV4	1768466	3573010	35.43%	2.333%
44	13.598	1971	1974	1978	rVB3	522316	626642	6.21%	0.409%
45	13.668	1981	1986	1990	rBV	1930957	3139700	31.14%	2.050%
46	13.739	1995	1998	2003	rVB3	595750	714123	7.08%	0.466%
47	13.863	2003	2019	2023	rBV2	2273473	5502996	54.57%	3.593%
48	13.904	2023	2026	2030	rVV2	910222	1234715	12.24%	0.806%
49	13.986	2035	2040	2046	rBV2	4961371	7858796	77.93%	5.131%
50	14.033	2046	2048	2050	rVV3	481649	603187	5.98%	0.394%
51	14.063	2050	2053	2060	rVV	846703	1863227	18.48%	1.217%
52	14.127	2060	2064	2066	rVV	854577	1381816	13.70%	0.902%
53	14.157	2066	2069	2073	rVV	1206206	1935177	19.19%	1.264%
54	14.210	2074	2078	2083	rVB	1537499	2306700	22.87%	1.506%
55	14.321	2091	2097	2102	rBV2	2150682	3626589	35.96%	2.368%
56	14.398	2102	2110	2114	rBV6	798732	1991055	19.74%	1.300%
57	14.451	2114	2119	2122	rBV6	479548	847635	8.41%	0.553%
58	14.498	2122	2127	2132	rBV3	2443726	4008079	39.75%	2.617%
59	14.574	2137	2140	2143	rVB	1025786	1261588	12.51%	0.824%
60	14.615	2143	2147	2151	rBV	1201614	1507787	14.95%	0.984%
61	14.662	2151	2155	2161	rVB3	1519196	2486316	24.66%	1.623%
62	14.721	2161	2165	2167	rBV	836452	1280832	12.70%	0.836%
63	14.757	2168	2171	2175	rVB	1266946	1653611	16.40%	1.080%
64	14.810	2175	2180	2181	rBV	1577224	2398974	23.79%	1.566%
65	14.927	2192	2200	2205	rBV3	2956156	7467057	74.05%	4.875%
66	14.974	2205	2208	2216	rVB3	1170291	1994283	19.78%	1.302%
67	15.080	2221	2226	2232	rVB	1744358	3061424	30.36%	1.999%
68	15.186	2240	2244	2249	rBV4	971501	1525118	15.12%	0.996%
69	15.310	2258	2265	2271	rVB4	1201488	2744978	27.22%	1.792%
70	15.462	2286	2291	2294	rBV6	520608	1003096	9.95%	0.655%
71	15.557	2302	2307	2311	rBV	961844	1581799	15.69%	1.033%
72	15.609	2311	2316	2320	rBV	1011581	1857272	18.42%	1.213%
73	15.692	2327	2330	2340	rVB3	968592	2125960	21.08%	1.388%
74	15.798	2340	2348	2356	rBV3	889246	2273896	22.55%	1.485%
75	15.880	2357	2362	2367	rVV2	274496	553662	5.49%	0.362%
76	15.974	2369	2378	2379	rVV4	561393	1322899	13.12%	0.864%

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ClientSampleId :
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Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Title : SW846 8260

77	16.009	2379	2384	2394	rVV	2014166	4189642	41.55%	2.736%
78	16.104	2396	2400	2405	rVV4	240745	470905	4.67%	0.307%
79	16.180	2407	2413	2428	rVB3	585446	2038397	20.21%	1.331%
80	16.339	2431	2440	2446	rBV	988494	2397648	23.78%	1.565%
81	16.539	2467	2474	2481	rBV2	955218	2124341	21.07%	1.387%
82	16.609	2481	2486	2500	rVB5	522401	1574215	15.61%	1.028%

Sum of corrected areas: 153155496

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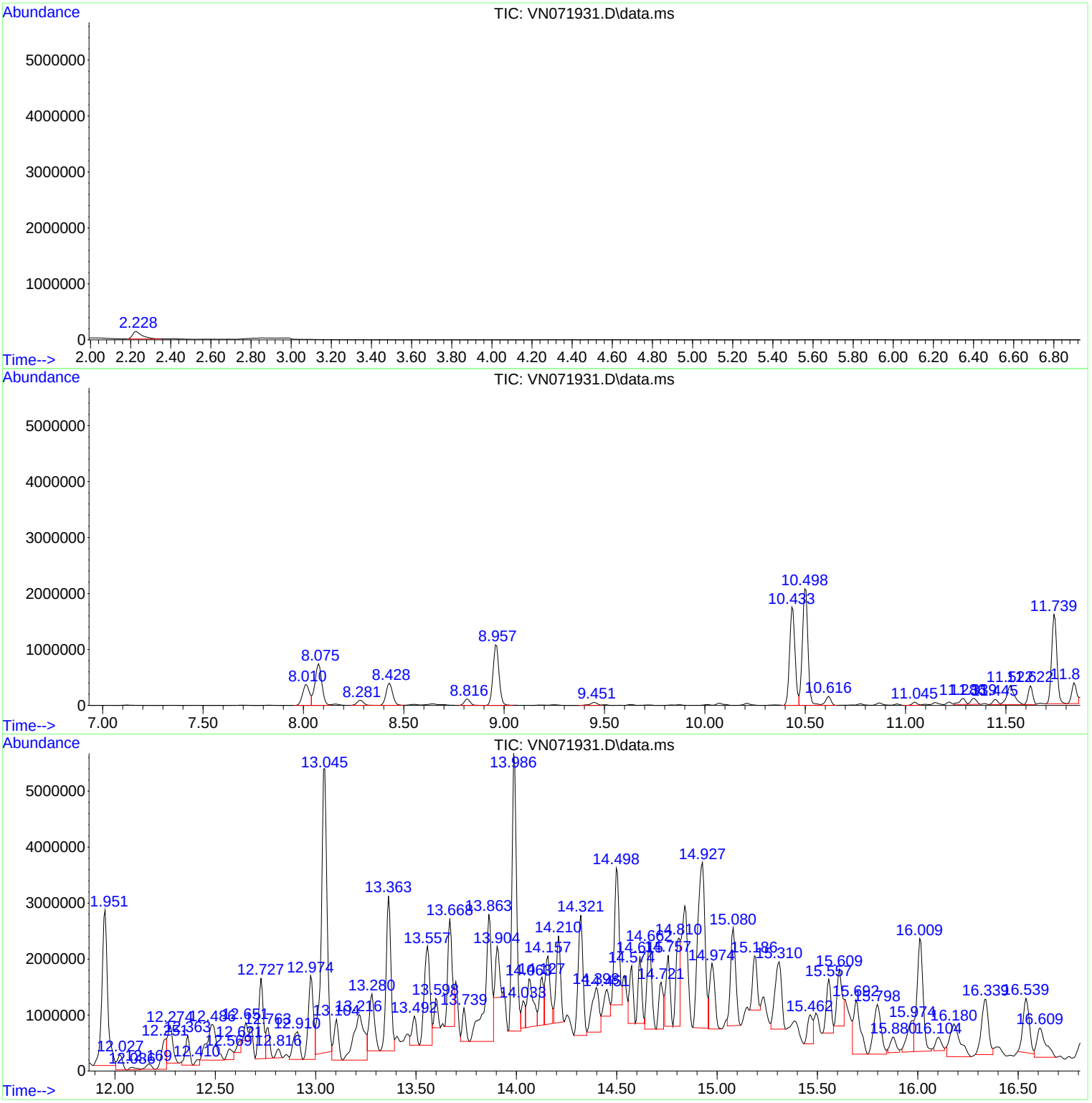
Instrument :
MSVOA_N
ClientSampleId :
2404-2405

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041122\
Data File : VN071931.D
Acq On : 11 Apr 2022 13:16
Operator : JC\MD
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

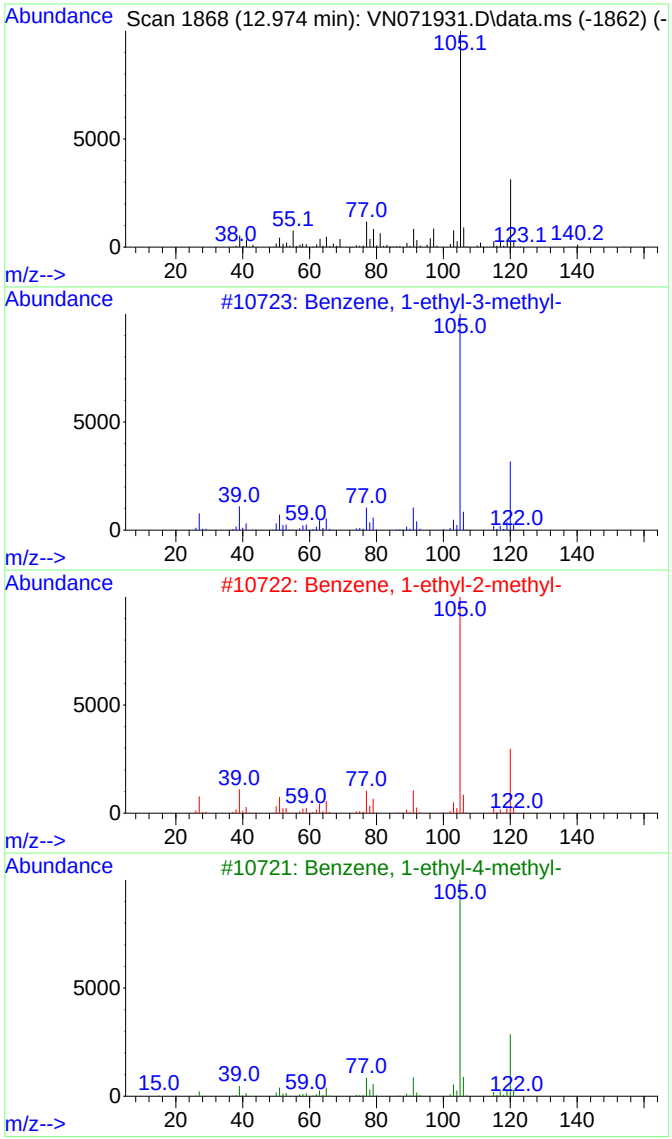
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

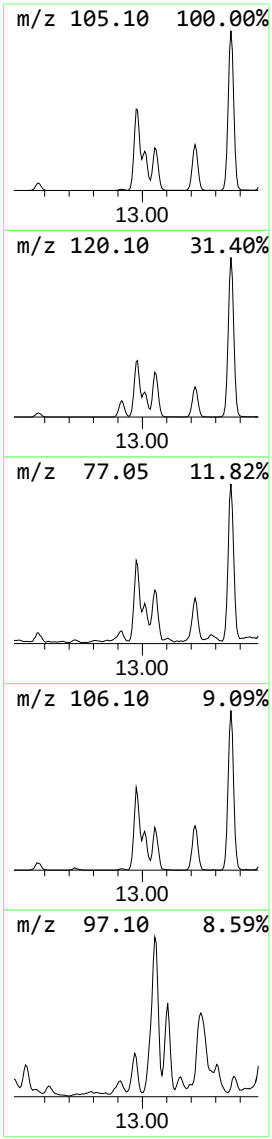
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Benzene, 1-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.974	43.68 ug/l	2742690	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	81
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	81





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Operator : JC\MD
Sample : N2306-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

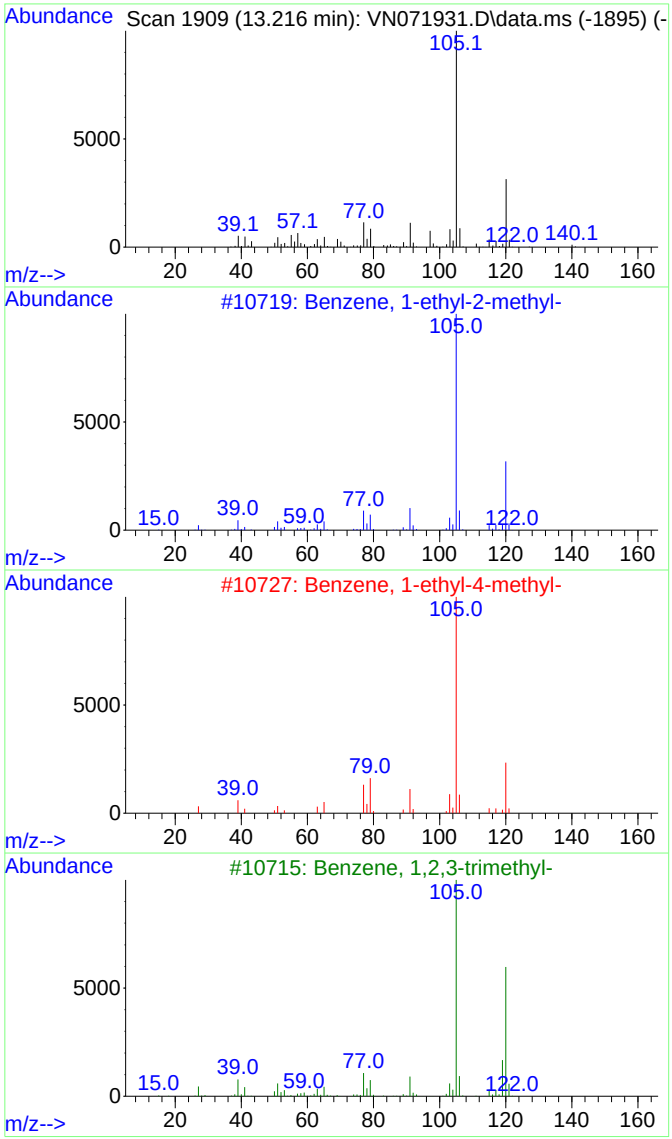
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

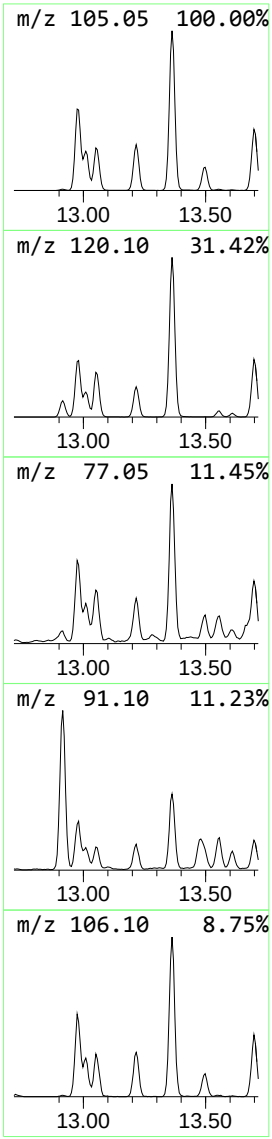
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	48.88 ug/l	3069390	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	87
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87





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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

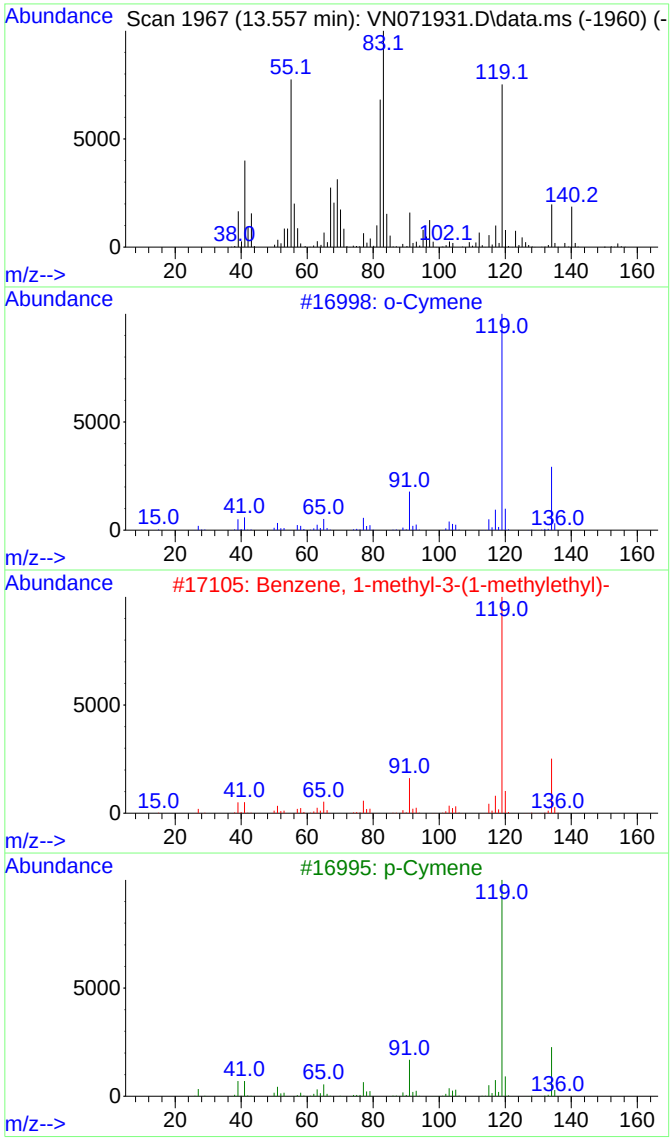
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

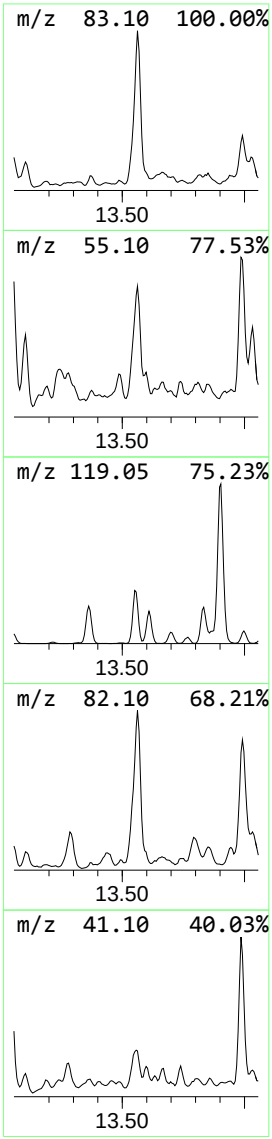
****

Peak Number 3 o-Cymene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.557	56.90 ug/l	3573010	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	78
2	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	78
3	p-Cymene	134	C10H14	000099-87-6	78
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	46
5	Cyclohexane, pentyl-	154	C11H22	004292-92-6	38





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Acq On : 11 Apr 2022 13:16
Operator : JC\MD
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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

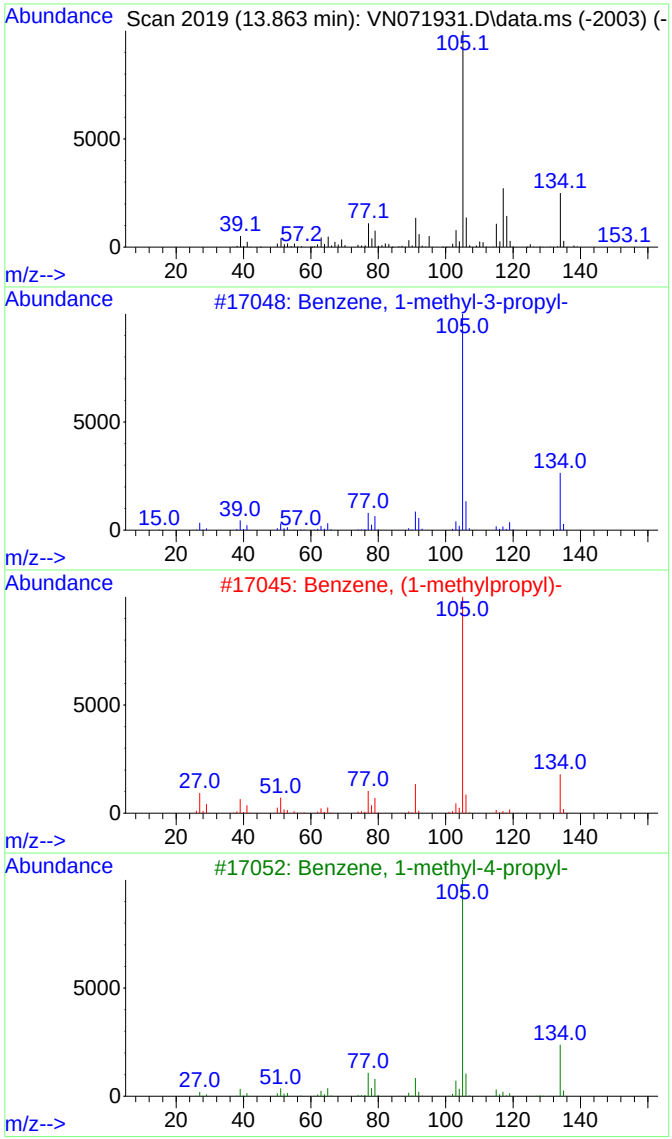
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

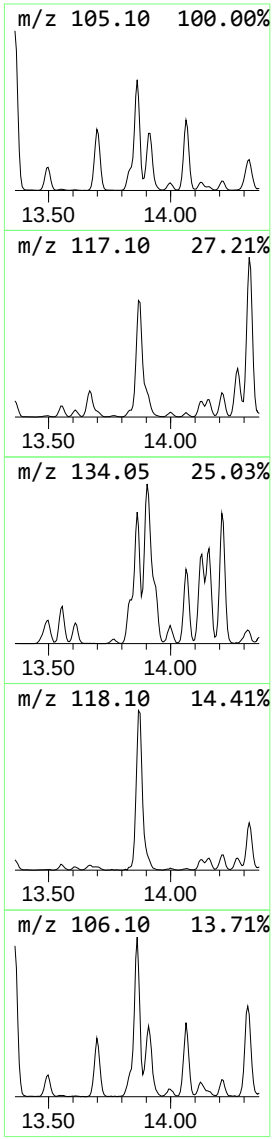
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-methyl-3-propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	87.64 ug/l	5503000	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	60
2	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	60
3	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	60
4	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	60
5	2-Indanol	134	C9H10O	004254-29-9	53





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Operator : JC\MD
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Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

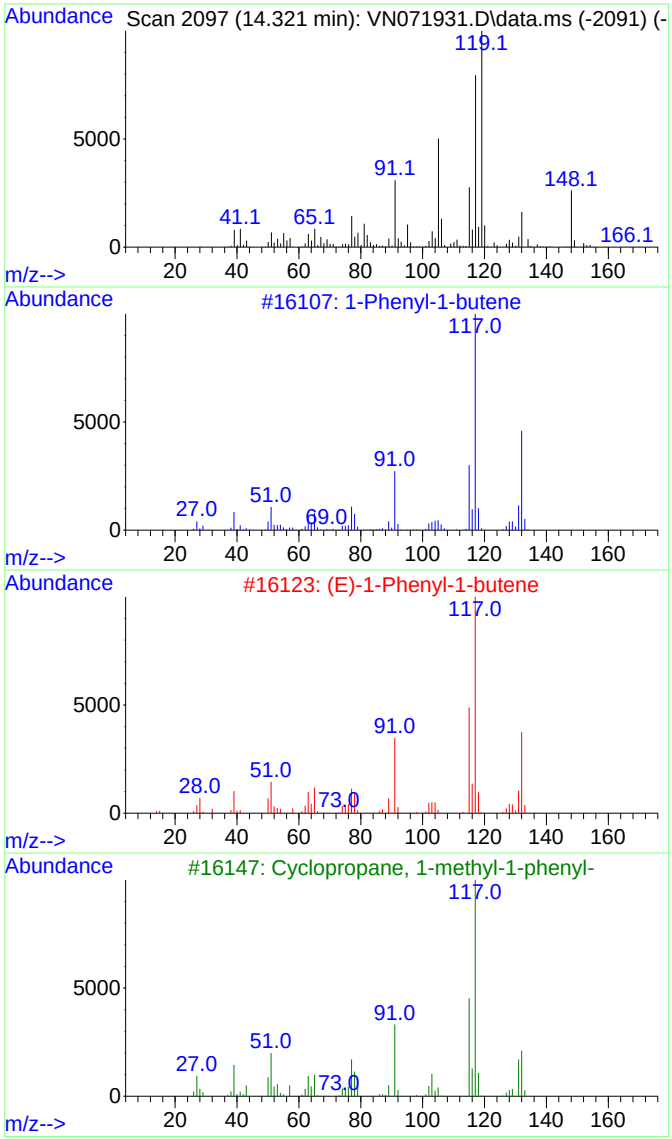
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

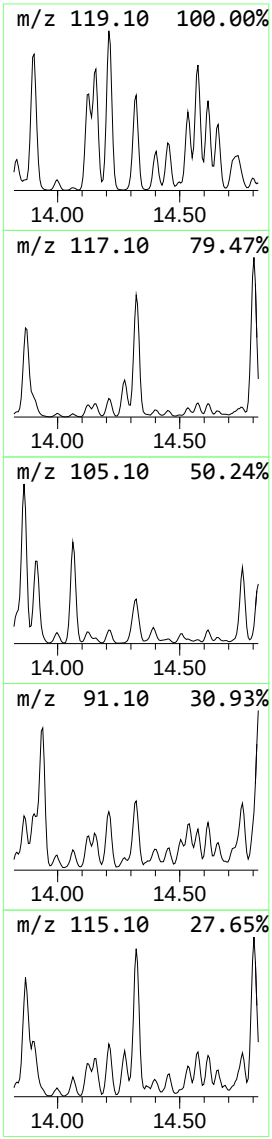
****

Peak Number 5 unknown14.321 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.321	57.75 ug/l	3626590	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	46
2	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	46
3	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	46
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	46
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	46





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MSVOA_N
ClientSampleId :
2404-2405

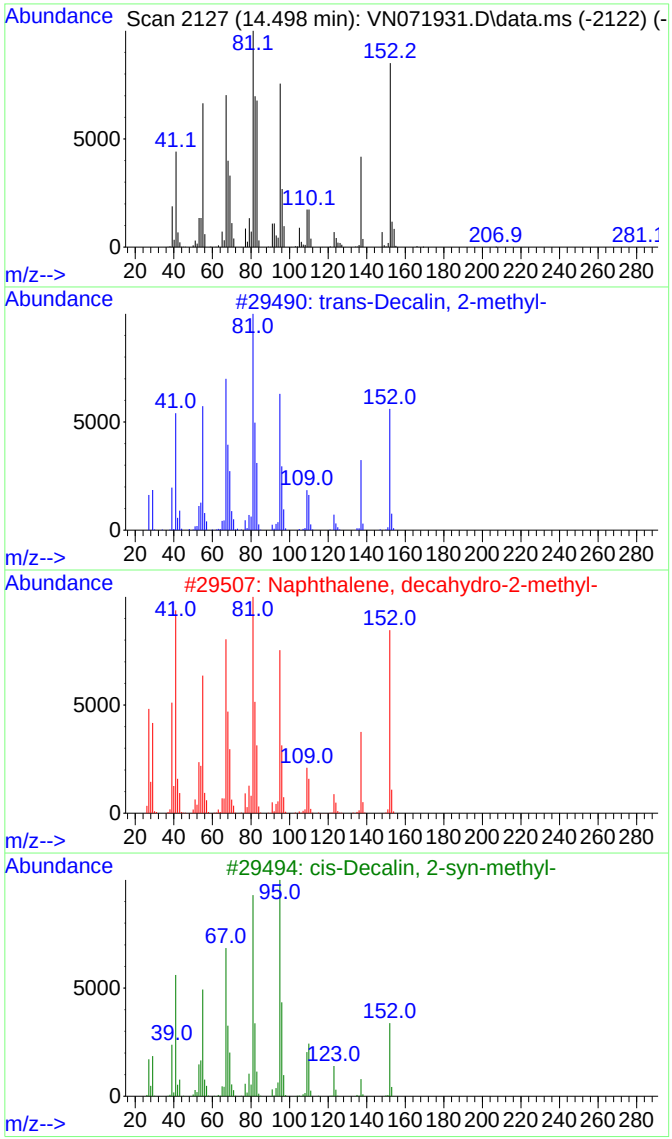
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

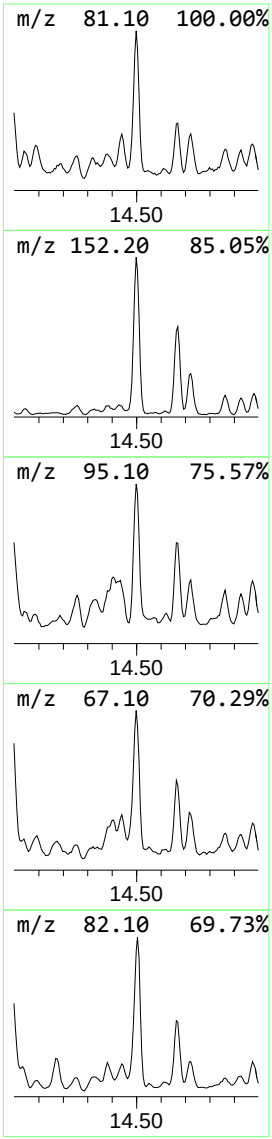
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 trans-Decalin, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	63.83 ug/l	4008080	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	97
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	95
3	cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	83
4	Cyclopentylcyclohexane	152	C11H20	001606-08-2	70
5	Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	58





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Acq On : 11 Apr 2022 13:16
Operator : JC\MD
Sample : N2306-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

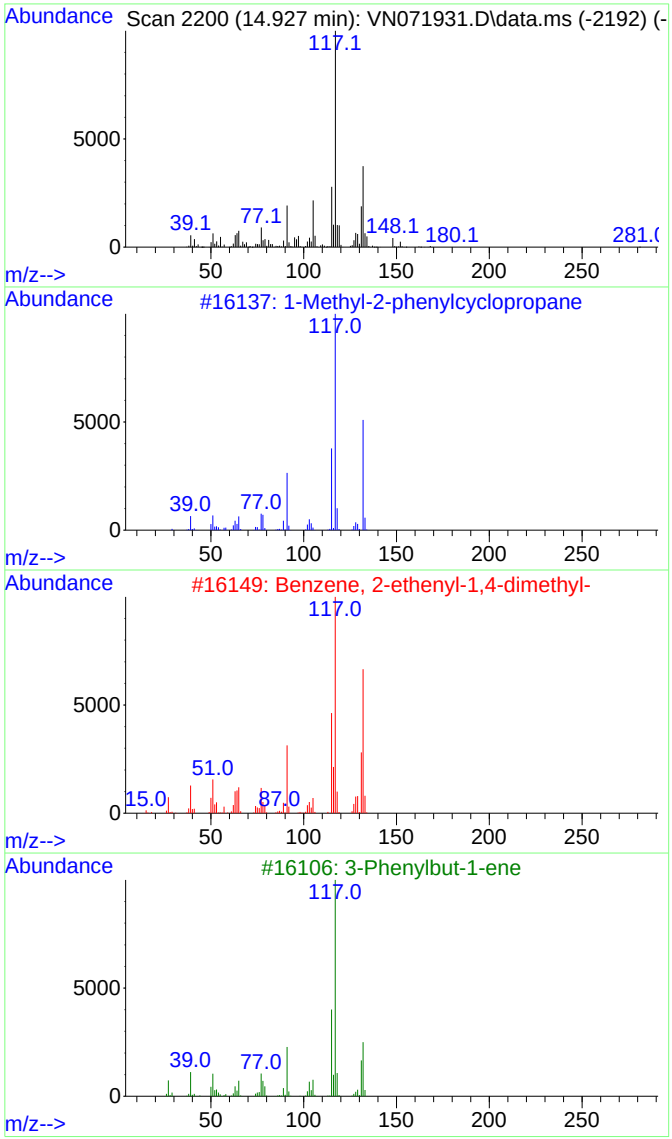
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

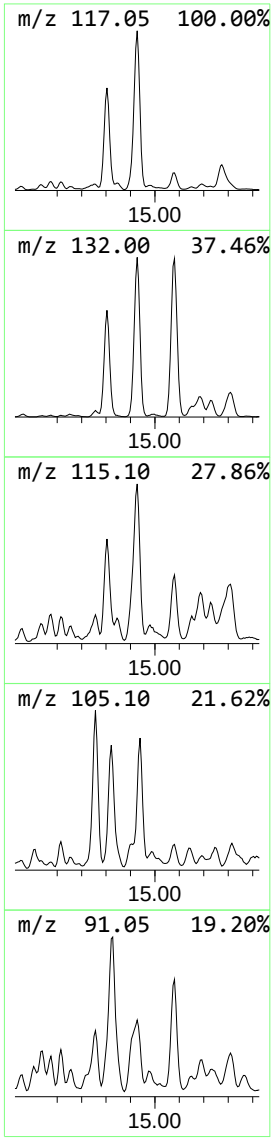
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Methyl-2-phenylcyclopropane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	118.91 ug/l	7467060	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	91
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
4	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81
5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	76





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Data File : VN071931.D
Acq On : 11 Apr 2022 13:16
Operator : JC\MD
Sample : N2306-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

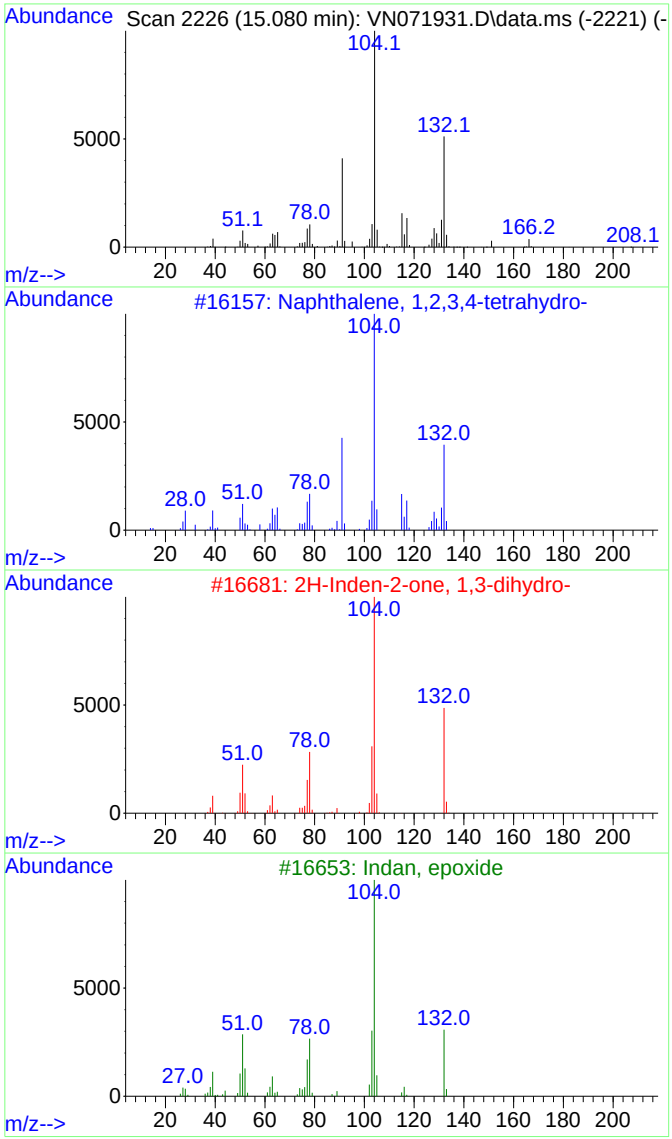
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

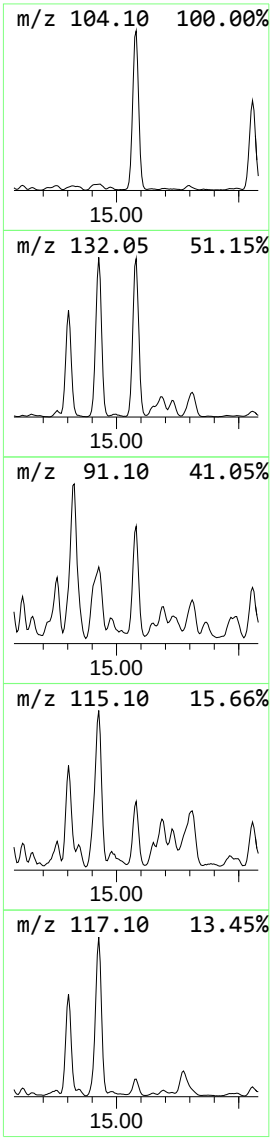
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.080	48.75 ug/l	3061420	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	62
3	Indan, epoxide	132	C9H8O	000768-22-9	50
4	Benzene, 3-cyclohexen-1-yl-	158	C12H14	004994-16-5	47
5	4-Cyanobenzoic acid, 2-phenyleth...	251	C16H13NO2	131786-46-4	38





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Data File : VN071931.D
Acq On : 11 Apr 2022 13:16
Operator : JC\MD
Sample : N2306-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

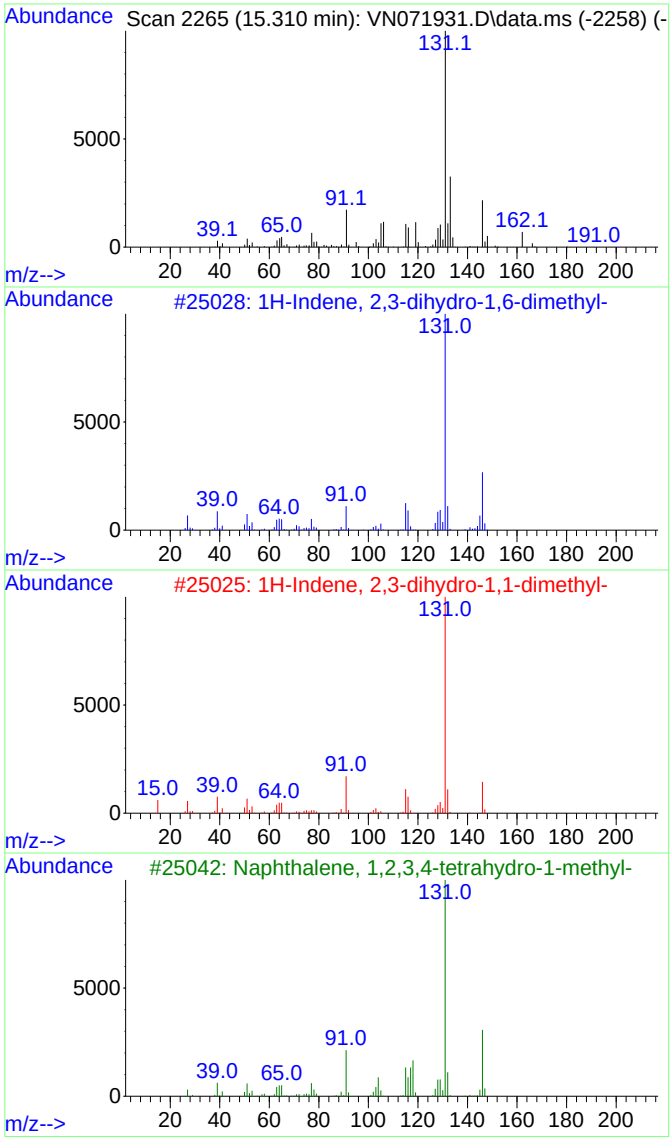
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

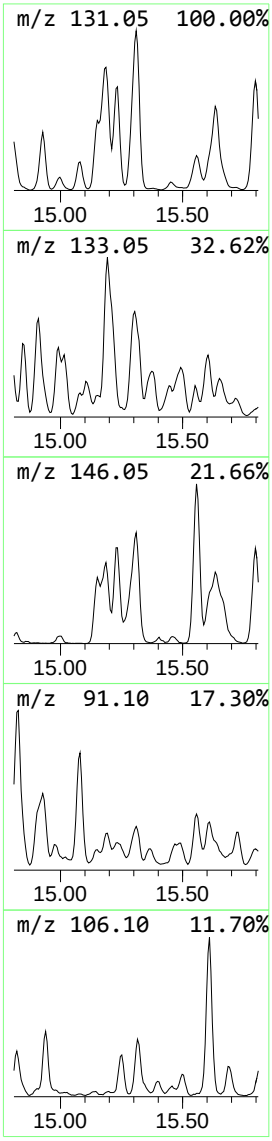
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Indene, 2,3-dihydro-1,6-... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	43.71 ug/l	2744980	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	92
2	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	70
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	70
4	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	70
5	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	70





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Data File : VN071931.D
Acq On : 11 Apr 2022 13:16
Operator : JC\MD
Sample : N2306-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

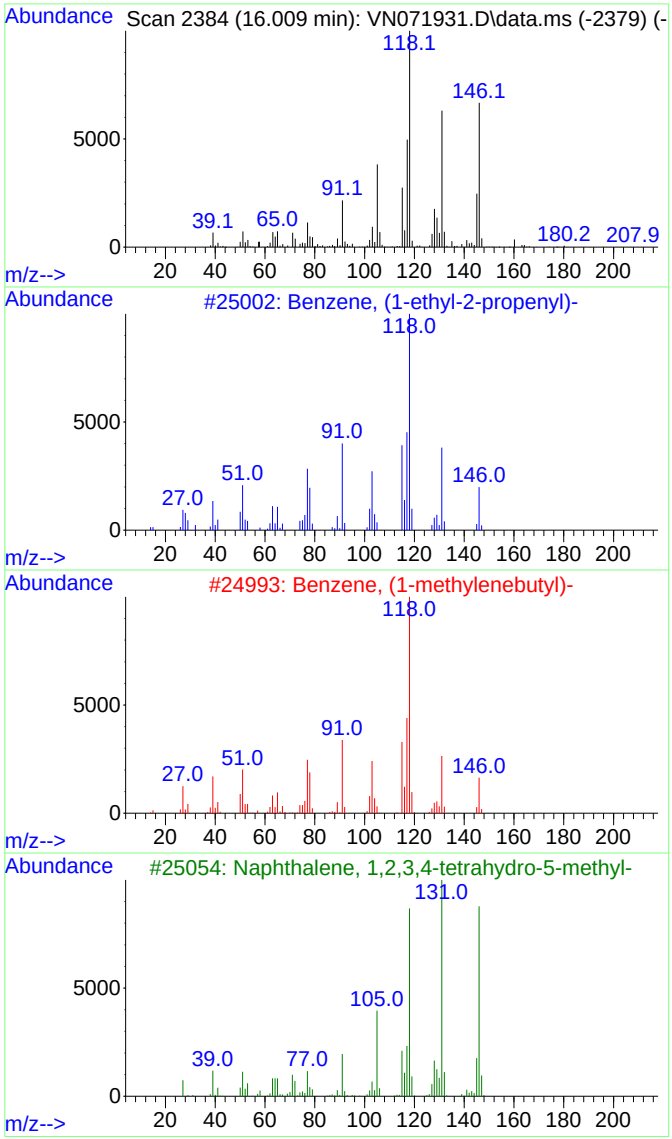
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

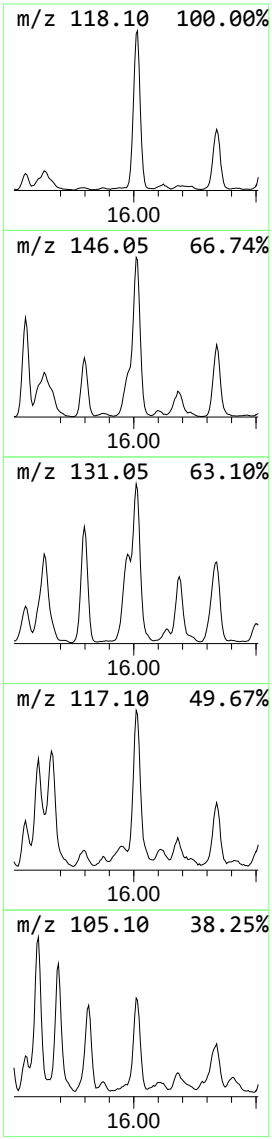
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, (1-ethyl-2-propenyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	66.72 ug/l	4189640	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	87
2	Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	87
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	74
4	1H-1,3,2-Benzodiazaborole, 2-eth...	146	C8H11BN2	074663-81-3	68
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041122\
Data File : VN071931.D
Acq On : 11 Apr 2022 13:16
Operator : JC\MD
Sample : N2306-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
2404-2405

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
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
Benzene, 1-ethy...	12.974	43.7	ug/l	2742690	4	13.668	3139700	50.0
Benzene, 1-ethy...	13.216	48.9	ug/l	3069390	4	13.668	3139700	50.0
o-Cymene	13.557	56.9	ug/l	3573010	4	13.668	3139700	50.0
Benzene, 1-meth...	13.863	87.6	ug/l	5503000	4	13.668	3139700	50.0
unknown14.321	14.321	57.8	ug/l	3626590	4	13.668	3139700	50.0
trans-Decalin, ...	14.498	63.8	ug/l	4008080	4	13.668	3139700	50.0
1-Methyl-2-phen...	14.927	118.9	ug/l	7467060	4	13.668	3139700	50.0
Naphthalene, 1,...	15.080	48.8	ug/l	3061420	4	13.668	3139700	50.0
1H-Indene, 2,3-...	15.310	43.7	ug/l	2744980	4	13.668	3139700	50.0
Benzene, (1-eth...	16.009	66.7	ug/l	4189640	4	13.668	3139700	50.0