LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040324\
Data File : VN081661.D
Acq On : 03 Apr 2024 16:11
Operator : JC\MD
Sample : P1952-12
Misc : 4.40g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-D-GRAB

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\82N031824W.M
Title : SW846 8260

Signal : TIC: VN081661.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.848	141	152	153	rBV5	56567	126184	2.14%	0.135%
2	8.165	1044	1056	1060	rBV	312196	736025	12.46%	0.785%
3	8.218	1060	1065	1077	rVB	553344	1239474	20.98%	1.323%
4	8.577	1116	1126	1136	rBV	316435	724042	12.25%	0.773%
5	9.100	1205	1215	1229	rBV	796126	1619146	27.40%	1.728%
6	9.594	1287	1299	1304	rBV5	29865	74761	1.27%	0.080%
7	10.565	1456	1464	1480	rBV	1255095	2307593	39.05%	2.462%
8	10.747	1489	1495	1502	rVB7	31630	81485	1.38%	0.087%
9	10.906	1518	1522	1530	rVB4	46727	86554	1.46%	0.092%
10	11.000	1530	1538	1547	rBV7	39661	104354	1.77%	0.111%
11	11.171	1559	1567	1574	rBV2	68460	126616	2.14%	0.135%
12	11.271	1574	1584	1592	rBV2	66311	156214	2.64%	0.167%
13	11.418	1602	1609	1614	rVV	88881	175299	2.97%	0.187%
14	11.471	1614	1618	1623	rVB	144570	239401	4.05%	0.255%
15	11.571	1631	1635	1639	rBV3	66330	105569	1.79%	0.113%
16	11.624	1639	1644	1645	rVV3	47466	76823	1.30%	0.082%
17	11.677	1649	1653	1660	rVB	84207	148335	2.51%	0.158%
18	11.741	1660	1664	1669	rBV2	48619	77710	1.32%	0.083%
19	11.865	1677	1685	1698	rBV	1001495	1836854	31.09%	1.960%
20	12.047	1711	1716	1721	rVB4	59385	125579	2.13%	0.134%
21	12.112	1721	1727	1730	rBV	187728	328013	5.55%	0.350%
22	12.153	1731	1734	1739	rVB4	145416	240889	4.08%	0.257%
23	12.212	1739	1744	1751	rBV7	33629	89846	1.52%	0.096%
24	12.288	1751	1757	1763	rBV6	85982	163620	2.77%	0.175%
25	12.371	1764	1771	1777	rBV4	306281	714999	12.10%	0.763%
26	12.482	1784	1790	1795	rVB4	372552	673515	11.40%	0.719%
27	12.588	1795	1808	1812	rBV4	359445	1319746	22.34%	1.408%
28	12.735	1829	1833	1836	rBV5	97923	178585	3.02%	0.191%
29	12.765	1836	1838	1842	rVB3	145942	188255	3.19%	0.201%
30	12.853	1847	1853	1860	rBV	874713	1478703	25.03%	1.578%
31	12.935	1861	1867	1872	rBV8	151250	322791	5.46%	0.344%
32	13.018	1877	1881	1888	rVB3	387259	722787	12.23%	0.771%
33	13.094	1888	1894	1899	rBV5	204219	462154	7.82%	0.493%
34	13.176	1899	1908	1913	rBV5	430388	1147361	19.42%	1.224%
35	13.224	1913	1916	1922	rVB5	245578	415302	7.03%	0.443%
36	13.312	1926	1931	1935	rBV2	210759	362920	6.14%	0.387%

LSC Area Percent Report

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ClientSampleId :
WC-D-GRAB

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
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Peak separation: 5

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Title : SW846 8260

37	13.359	1935	1939	1942	rBV2	180701	273130	4.62%	0.291%
38	13.400	1942	1946	1952	rVB5	296825	474813	8.04%	0.507%
39	13.523	1959	1967	1971	rBV3	269591	639509	10.82%	0.682%
40	13.576	1972	1976	1980	rVV3	311341	550774	9.32%	0.588%
41	13.612	1980	1982	1986	rVV4	170075	295616	5.00%	0.315%
42	13.682	1987	1994	1998	rVV4	594198	1463138	24.76%	1.561%
43	13.718	1998	2000	2004	rVV3	345074	474480	8.03%	0.506%
44	13.794	2008	2013	2022	rVB	1036489	1956063	33.11%	2.087%
45	13.947	2032	2039	2050	rBV5	498491	1139238	19.28%	1.216%
46	14.035	2051	2054	2057	rBV2	123419	156437	2.65%	0.167%
47	14.118	2062	2068	2073	rBV3	1105942	2170459	36.73%	2.316%
48	14.218	2080	2085	2089	rBV5	306247	548626	9.29%	0.585%
49	14.259	2089	2092	2095	rVV4	124712	177129	3.00%	0.189%
50	14.329	2100	2104	2113	rVB	1124902	2138580	36.19%	2.282%
51	14.441	2117	2123	2129	rVB3	555332	1213069	20.53%	1.294%
52	14.506	2129	2134	2139	rBV7	361324	687909	11.64%	0.734%
53	14.629	2149	2155	2159	rBV2	1249037	1860822	31.49%	1.986%
54	14.735	2168	2173	2177	rBV	764377	1201386	20.33%	1.282%
55	14.800	2177	2184	2188	rVV4	966079	1849009	31.29%	1.973%
56	14.841	2188	2191	2196	rVV3	304597	538410	9.11%	0.575%
57	14.941	2204	2208	2210	rBV3	232878	376819	6.38%	0.402%
58	14.970	2211	2213	2218	rVV2	413349	622990	10.54%	0.665%
59	15.053	2219	2227	2231	rVV3	1099790	2737278	46.33%	2.921%
60	15.106	2231	2236	2245	rVB2	1054784	2233029	37.79%	2.383%
61	15.229	2253	2257	2260	rBV5	274957	468161	7.92%	0.500%
62	15.276	2260	2265	2268	rVV5	754648	1545813	26.16%	1.649%
63	15.317	2268	2272	2276	rVV2	1139237	2300217	38.93%	2.454%
64	15.365	2276	2280	2286	rVV3	909701	1964670	33.25%	2.096%
65	15.435	2286	2292	2299	rVB4	1754258	4268611	72.24%	4.555%
66	15.600	2315	2320	2329	rVB6	924742	1919289	32.48%	2.048%
67	15.700	2329	2337	2341	rBV2	1336608	3328260	56.33%	3.551%
68	15.794	2349	2353	2371	rVB10	1601534	5908623	100.00%	6.305%
69	15.947	2371	2379	2386	rBV2	1627237	4017191	67.99%	4.287%
70	16.023	2387	2392	2398	rBV2	572333	1392059	23.56%	1.485%
71	16.117	2402	2408	2420	rVB4	1331664	4144554	70.14%	4.423%
72	16.223	2421	2426	2427	rBV4	332969	570880	9.66%	0.609%
73	16.259	2428	2432	2437	rVB3	995705	1762344	29.83%	1.881%
74	16.329	2438	2444	2451	rBV4	1138972	3316682	56.13%	3.539%
75	16.500	2464	2473	2479	rBV4	1753540	5221236	88.37%	5.571%
76	16.712	2499	2509	2516	rVB4	2209302	5857376	99.13%	6.250%

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Title : SW846 8260

77	16.782	2516	2521	2522	rBV	696356	972801	16.46%	1.038%

Sum of corrected areas: 93714984

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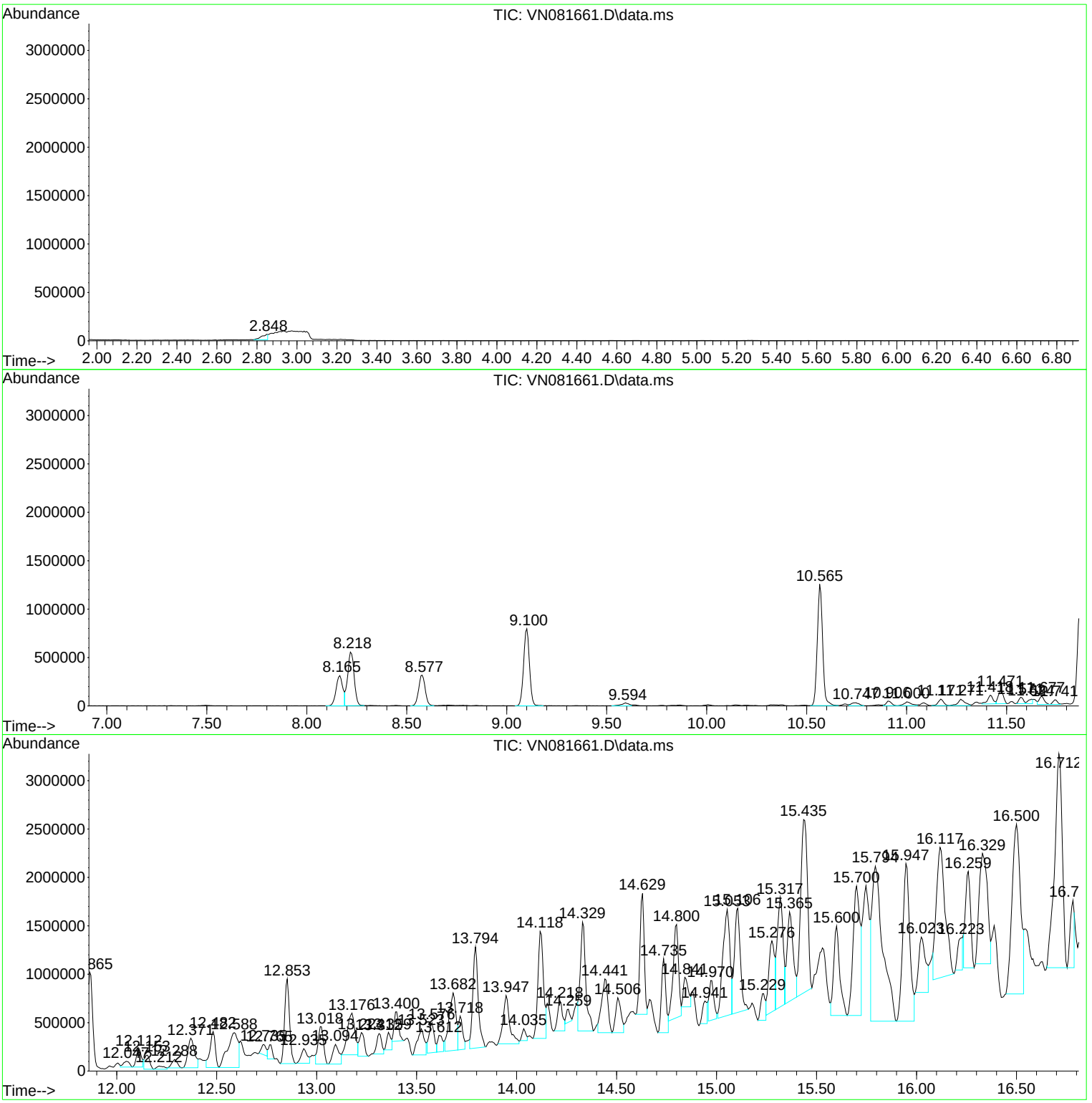
WC-D-GRAB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040324\
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MSVOA_N
ClientSampleId :
WC-D-GRAB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

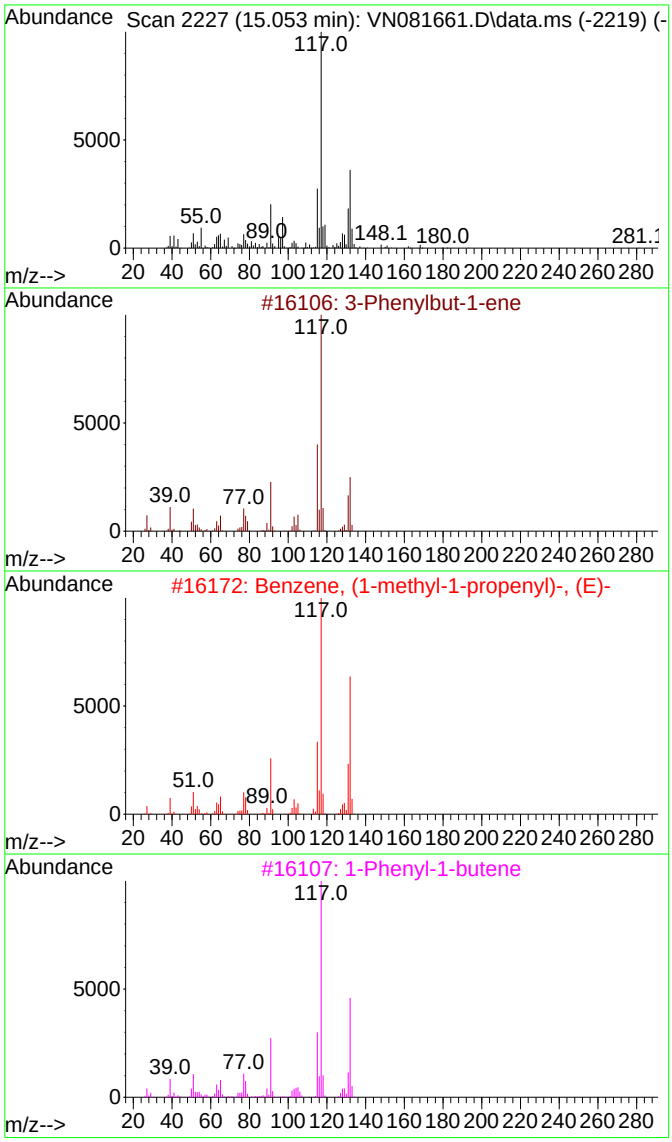
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

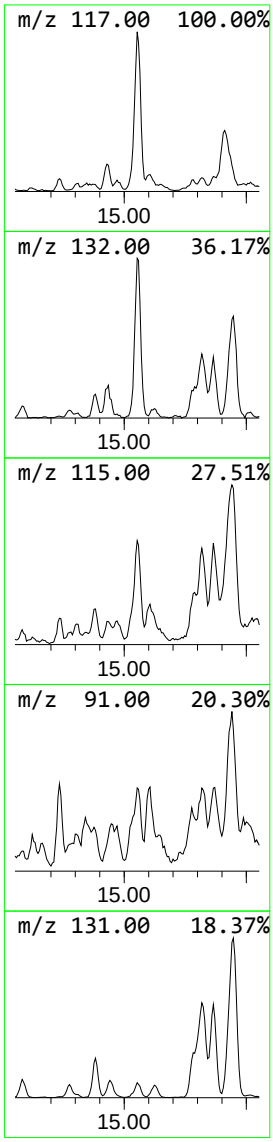
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	69.97 ug/l	2737280	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	83
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	80
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	80
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	74





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ClientSampleId :
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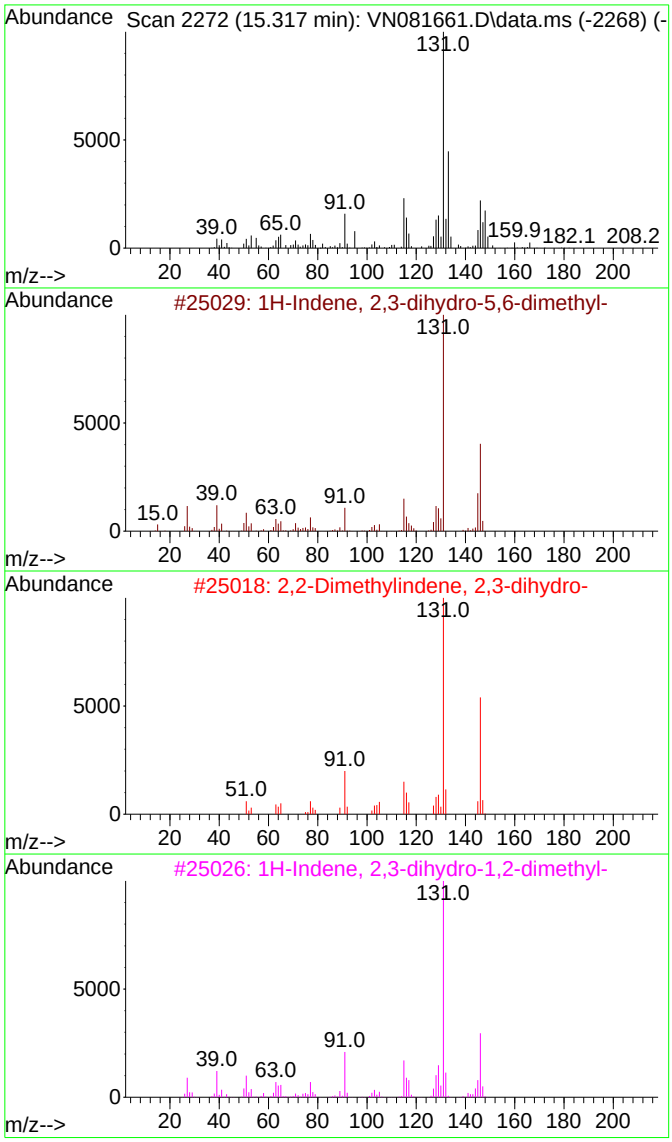
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

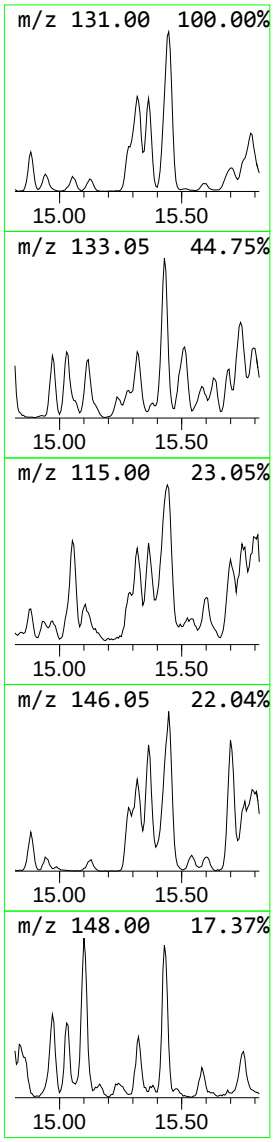
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1H-Indene, 2,3-dihydro-5,6-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.318	58.80 ug/l	2300220	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	70
2	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	70
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	70
4	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	70
5	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	70





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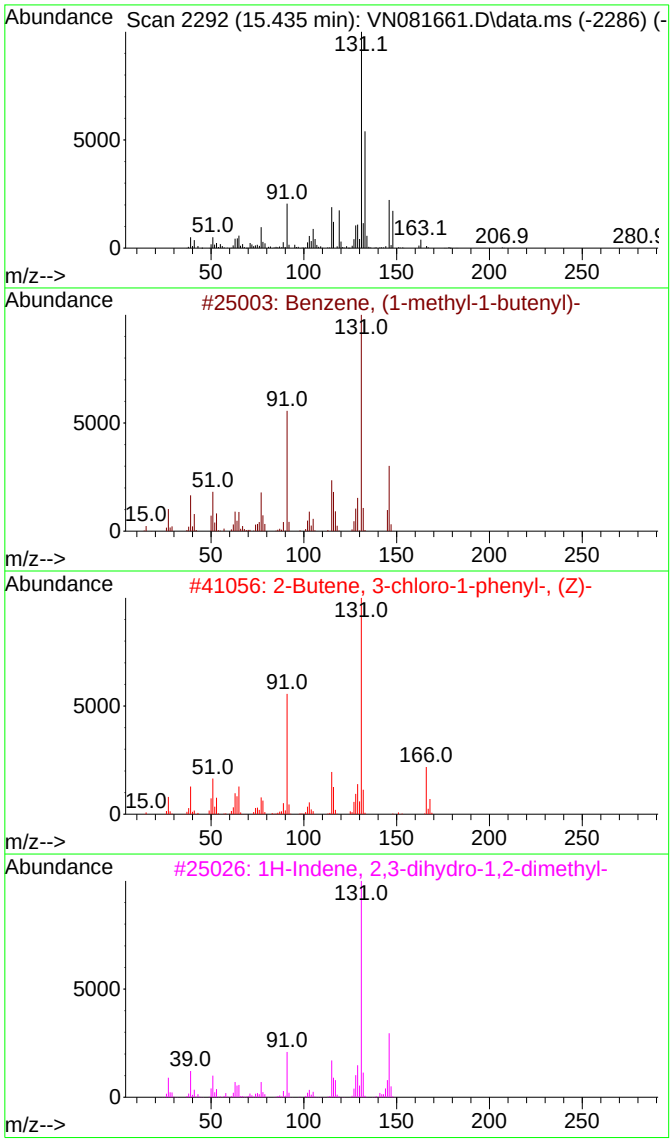
Quant Title : SW846 8260

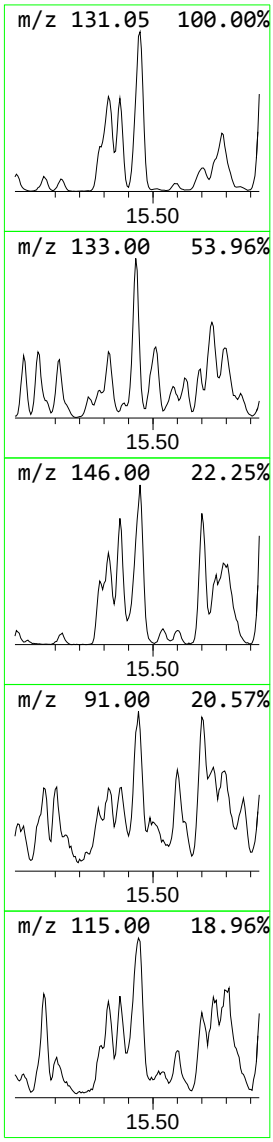
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, (1-methyl-1-butenyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.435	109.11 ug/l	4268610	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	91
2	2-Butene, 3-chloro-1-phenyl-, (Z)-	166	C10H11Cl	016608-68-7	87
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	64
4	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	64
5	1H-Indene, 2,3-dihydro-1,3-dimet...	146	C11H14	004175-53-5	64





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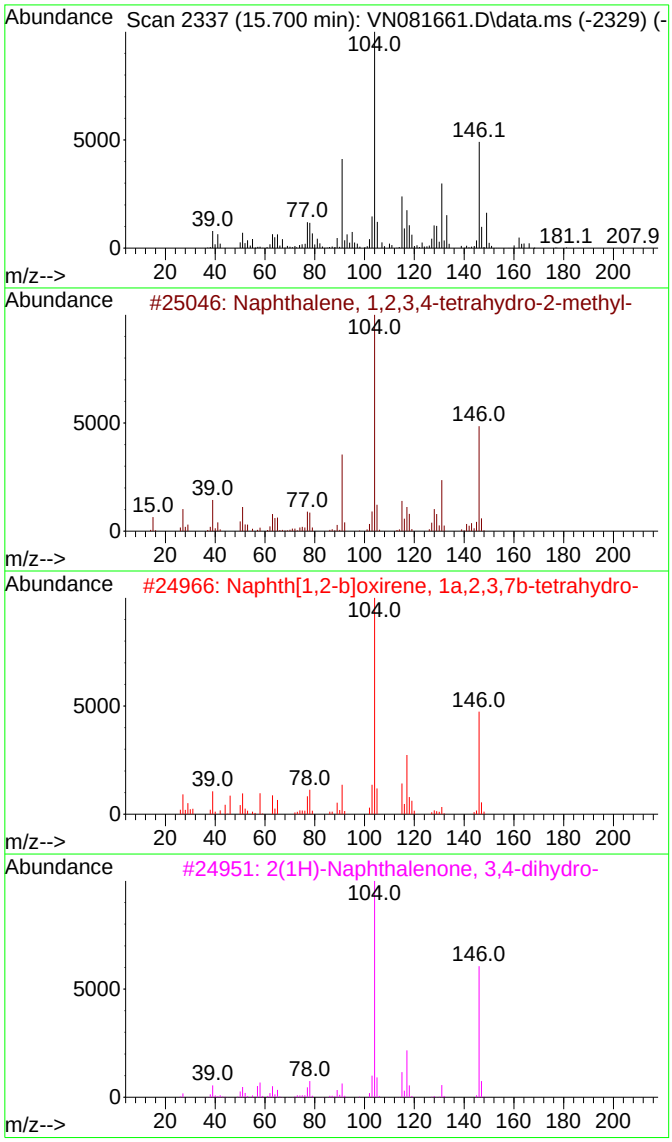
Quant Title : SW846 8260

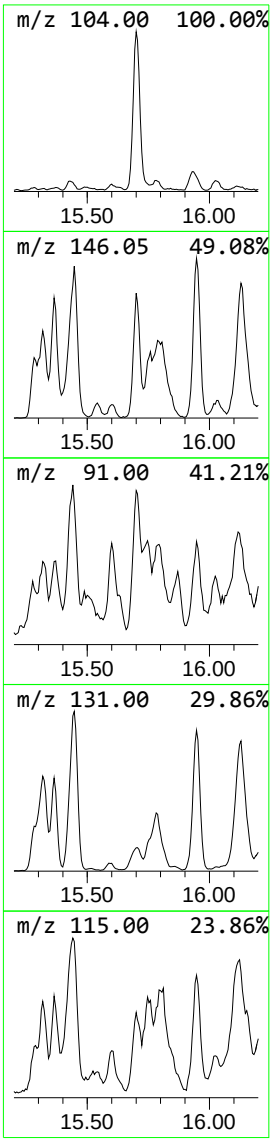
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.700	85.08 ug/l	3328260	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	003877-19-8	91
2	Naphth[1,2-b]oxirene, 1a,2,3,7b-...	146	C10H10O	002461-34-9	58
3	2(1H)-Naphthalenone, 3,4-dihydro-	146	C10H10O	000530-93-8	58
4	Naphthalene, 2-ethyl-1,2,3,4-tet...	160	C12H16	032367-54-7	47
5	7-Azabicyclo[4.2.2]deca-2,4,9-tr...	147	C9H9NO	017198-06-0	43





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Quant Title : SW846 8260

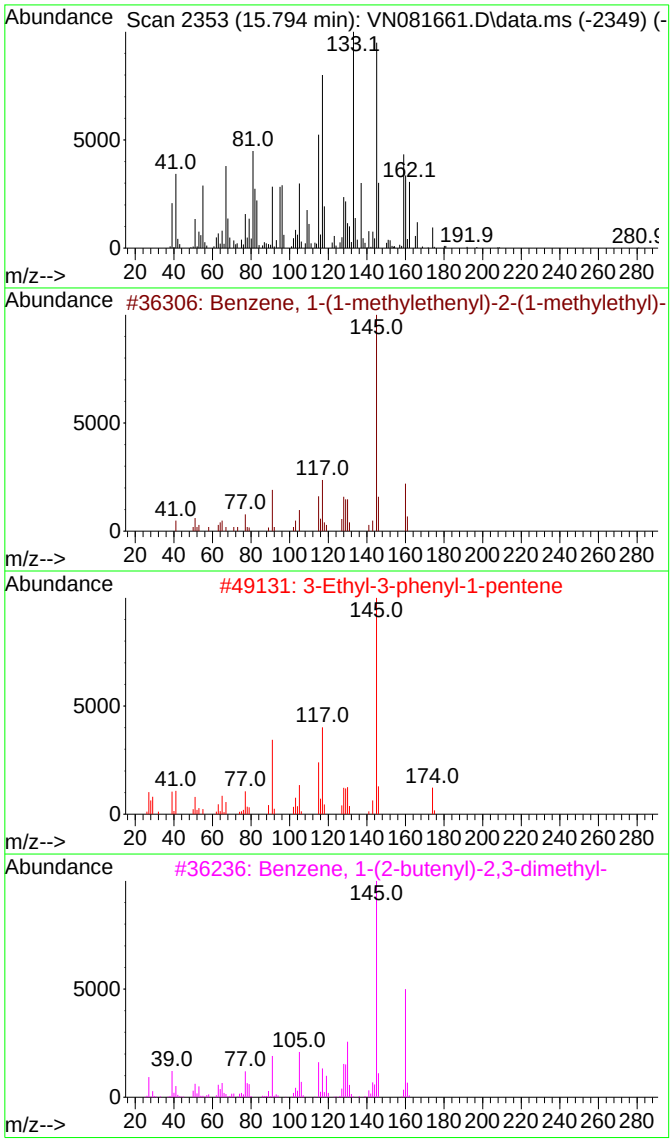
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

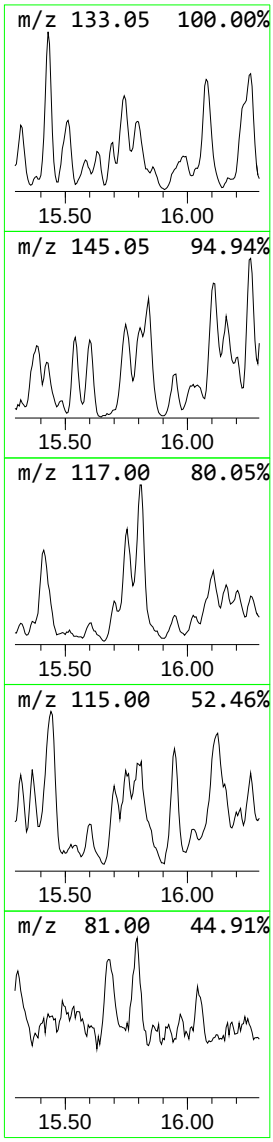
****

Peak Number 5 unknown15.794 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.794	151.03 ug/l	5908620	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	49
2	3-Ethyl-3-phenyl-1-pentene	174	C13H18	019781-34-1	45
3	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	38
4	1-Propanone, 1-(2,4-dimethylphen...	162	C11H14O	035031-55-1	25
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	25





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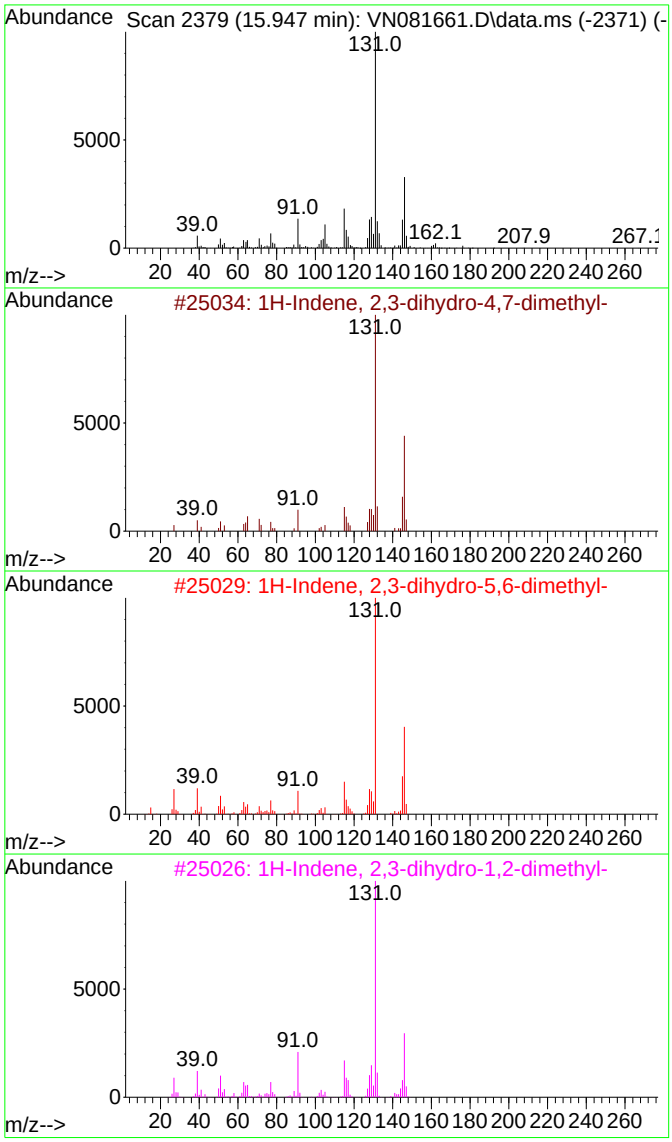
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

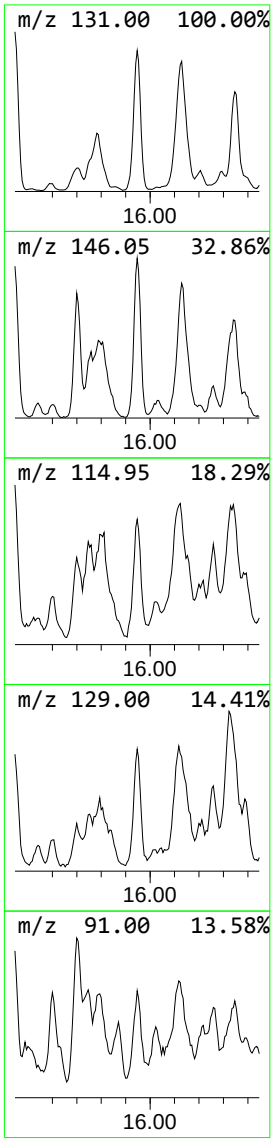
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.947	102.69 ug/l	4017190	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	96
2	1H-Indene, 2,3-dihydro-5,6-dimet...	146	C11H14	001075-22-5	94
3	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	94
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	94
5	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	93





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Data File : VN081661.D
Acq On : 03 Apr 2024 16:11
Operator : JC\MD
Sample : P1952-12
Misc : 4.40g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-D-GRAB

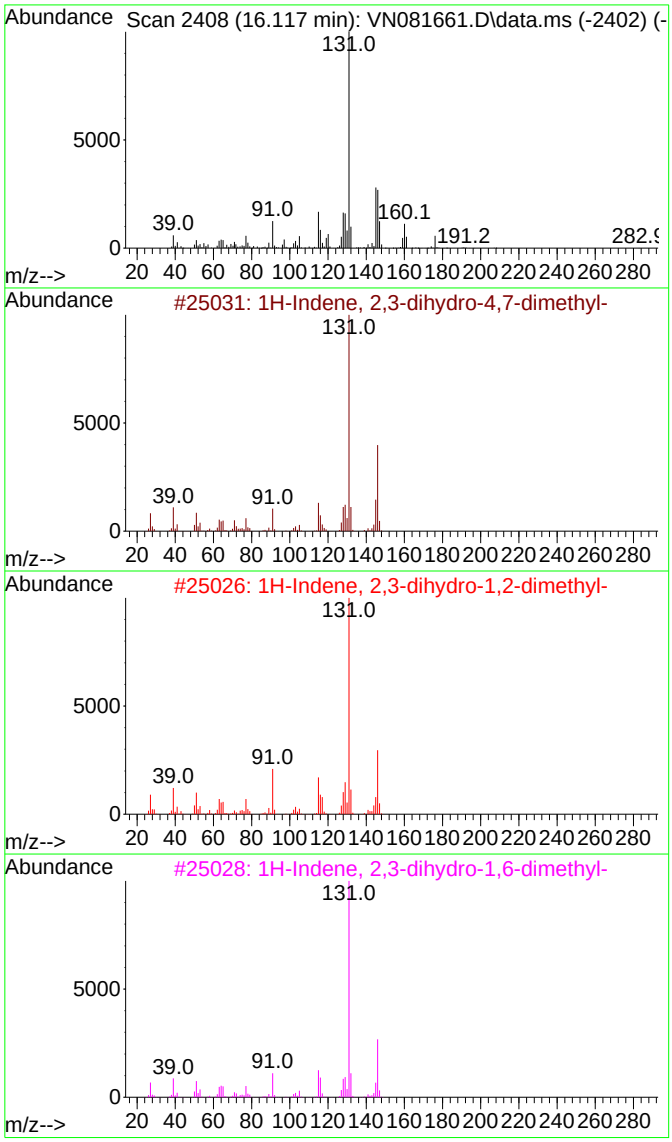
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

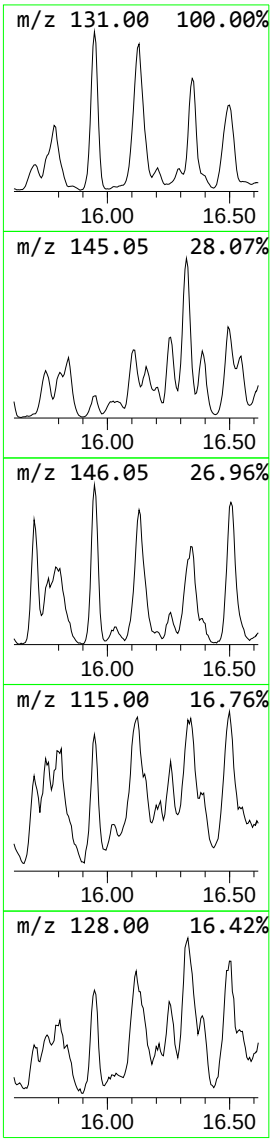
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.117	105.94 ug/l	4144550	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	81
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	76
3	1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	76
4	Benzene, (1,2-dimethyl-1-propenyl)-	146	C11H14	000769-57-3	76
5	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	68





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040324\
Data File : VN081661.D
Acq On : 03 Apr 2024 16:11
Operator : JC\MD
Sample : P1952-12
Misc : 4.40g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-D-GRAB

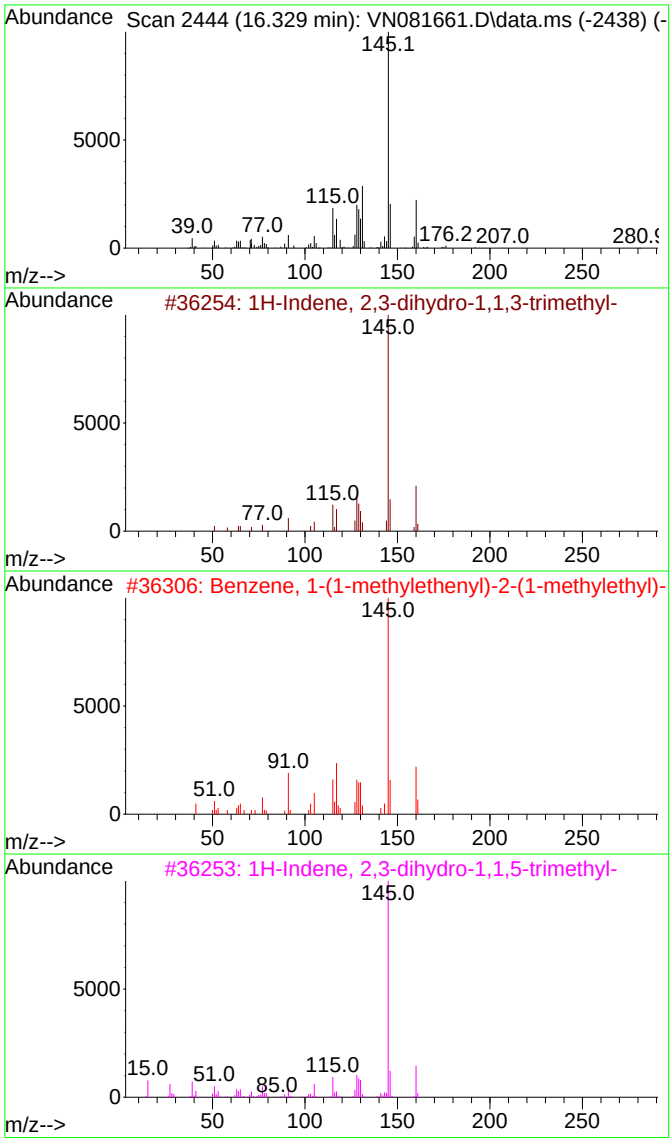
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

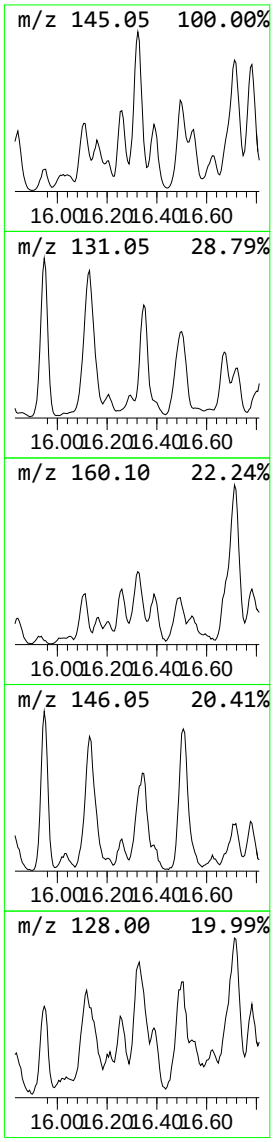
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.329	84.78 ug/l	3316680	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	87
2	Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	87
3	1H-Indene, 2,3-dihydro-1,1,5-tri...	160	C12H16	040650-41-7	81
4	Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	76
5	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	74





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Data File : VN081661.D
Acq On : 03 Apr 2024 16:11
Operator : JC\MD
Sample : P1952-12
Misc : 4.40g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-D-GRAB

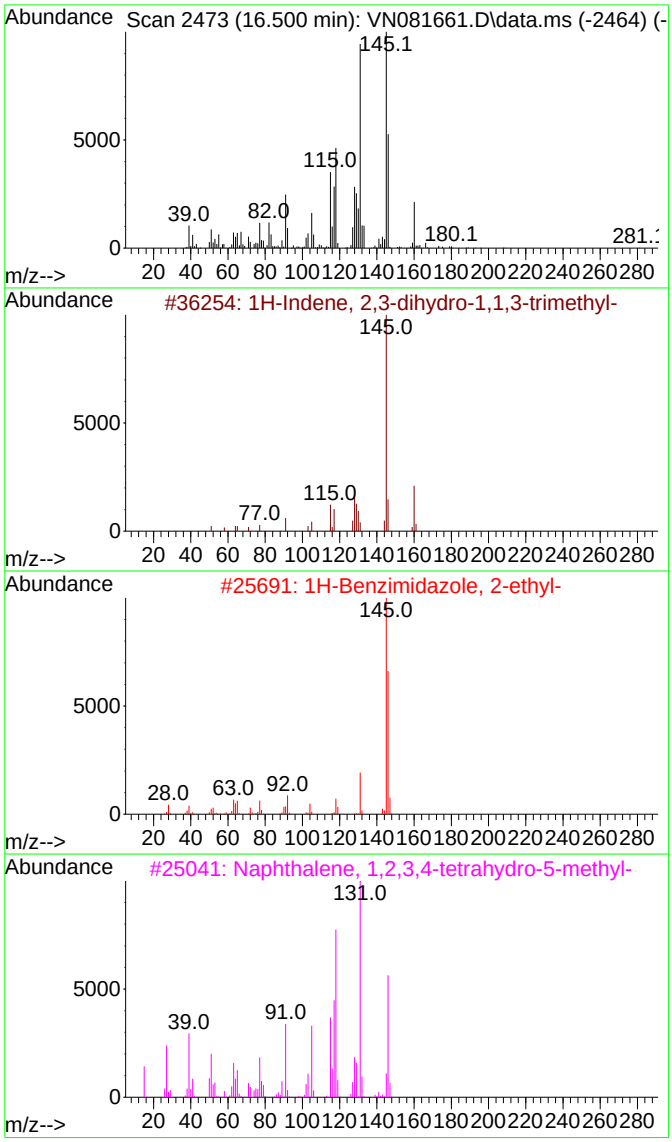
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

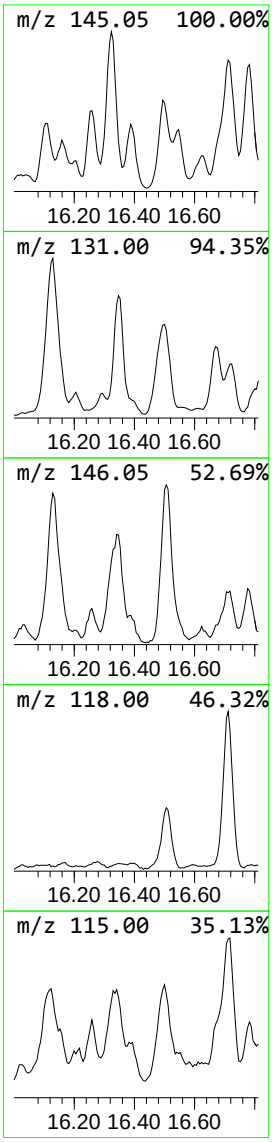
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1H-Benzimidazole, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.500	133.46 ug/l	5221240	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	64
2	1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	62
3	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	52
4	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	49
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040324\
Data File : VN081661.D
Acq On : 03 Apr 2024 16:11
Operator : JC\MD
Sample : P1952-12
Misc : 4.40g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-D-GRAB

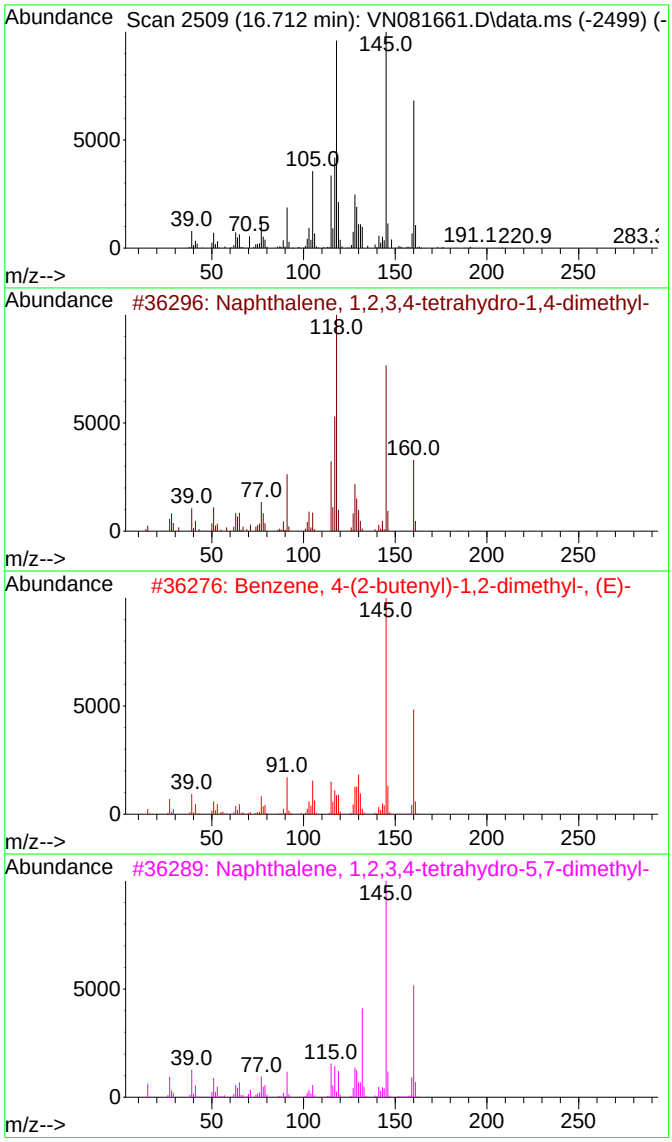
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.M
Quant Title : SW846 8260

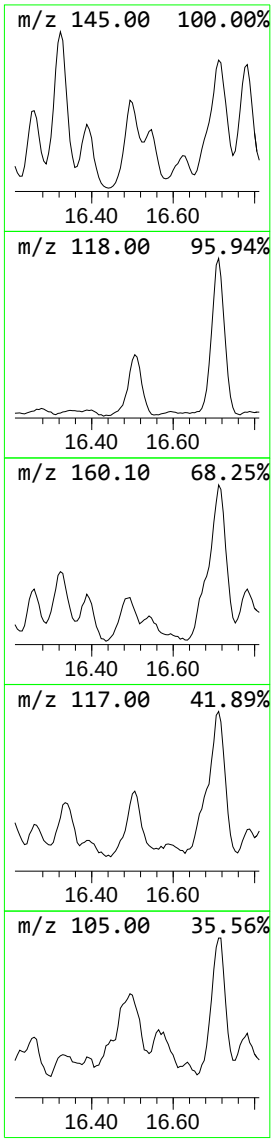
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.712	149.72 ug/l	5857380	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	95
2	Benzene, 4-(2-butenyl)-1,2-dimet...	160	C12H16	054340-86-2	86
3	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021693-54-9	83
4	Benzene, 1-(2-butenyl)-2,3-dimet...	160	C12H16	054340-85-1	78
5	Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040324\
Data File : VN081661.D
Acq On : 03 Apr 2024 16:11
Operator : JC\MD
Sample : P1952-12
Misc : 4.40g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-D-GRAB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031824W.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
3-Phenylbut-1-ene	15.053	70.0	ug/l	2737280	4	13.794	1956060	50.0
1H-Indene, 2,3-...	15.318	58.8	ug/l	2300220	4	13.794	1956060	50.0
Benzene, (1-met...	15.435	109.1	ug/l	4268610	4	13.794	1956060	50.0
Naphthalene, 1,...	15.700	85.1	ug/l	3328260	4	13.794	1956060	50.0
unknown15.794	15.794	151.0	ug/l	5908620	4	13.794	1956060	50.0
1H-Indene, 2,3-...	15.947	102.7	ug/l	4017190	4	13.794	1956060	50.0
1H-Indene, 2,3-...	16.117	105.9	ug/l	4144550	4	13.794	1956060	50.0
1H-Indene, 2,3-...	16.329	84.8	ug/l	3316680	4	13.794	1956060	50.0
1H-Benzimidazol...	16.500	133.5	ug/l	5221240	4	13.794	1956060	50.0
Naphthalene, 1,...	16.712	149.7	ug/l	5857380	4	13.794	1956060	50.0