LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121323\
Data File : VN080467.D
Acq On : 13 Dec 2023 17:16
Operator : JC\MD
Sample : 05791-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
597-A-J

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\82N121223W.M
Title : SW846 8260

Signal : TIC: VN080467.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.083	16	22	27	rBV2	25857	39140	2.56%	0.300%
2	2.483	86	90	100	rVB4	9572	23288	1.52%	0.178%
3	2.659	115	120	127	rVB	20063	38520	2.52%	0.295%
4	3.248	210	220	230	rVB5	6319	17739	1.16%	0.136%
5	3.653	281	289	297	rVV4	5958	17974	1.17%	0.138%
6	4.430	413	421	432	rBV2	7592	24396	1.59%	0.187%
7	7.324	905	913	926	rVB2	34371	98998	6.47%	0.758%
8	7.965	1012	1022	1035	rVB	68776	167045	10.91%	1.279%
9	8.165	1046	1056	1061	rBV	191709	464808	30.36%	3.558%
10	8.224	1061	1066	1080	rVB3	363993	953788	62.30%	7.300%
11	8.582	1118	1127	1142	rVB2	200274	595712	38.91%	4.560%
12	8.735	1145	1153	1159	rBV5	20750	50540	3.30%	0.387%
13	8.859	1167	1174	1181	rVB5	11561	24429	1.60%	0.187%
14	9.100	1204	1215	1231	rBV	526620	1089259	71.15%	8.337%
15	9.600	1291	1300	1308	rVB3	64572	146342	9.56%	1.120%
16	10.571	1456	1465	1471	rBV	695779	1306351	85.33%	9.999%
17	10.629	1471	1475	1485	rVB	179799	331871	21.68%	2.540%
18	11.865	1677	1685	1696	rBV	801769	1434357	93.69%	10.979%
19	11.965	1696	1702	1710	rVB	119954	201671	13.17%	1.544%
20	12.070	1712	1720	1733	rBV	472698	926288	60.50%	7.090%
21	12.400	1768	1776	1786	rBV	238240	402509	26.29%	3.081%
22	12.694	1821	1826	1834	rVB	43477	70647	4.61%	0.541%
23	12.847	1845	1852	1862	rBV	578692	993004	64.86%	7.600%
24	13.029	1877	1883	1889	rBV2	19791	33308	2.18%	0.255%
25	13.100	1889	1895	1898	rVV	80937	145578	9.51%	1.114%
26	13.129	1898	1900	1904	rVV2	57572	84180	5.50%	0.644%
27	13.176	1904	1908	1913	rVV	63411	96926	6.33%	0.742%
28	13.335	1929	1935	1943	rVV	80597	133313	8.71%	1.020%
29	13.482	1954	1960	1970	rVB	131956	220283	14.39%	1.686%
30	13.670	1987	1992	1997	rBV2	13996	22203	1.45%	0.170%
31	13.729	1997	2002	2006	rBV	16227	21711	1.42%	0.166%
32	13.794	2006	2013	2023	rVV2	830911	1530942	100.00%	11.718%
33	13.876	2023	2027	2034	rVB5	12768	24857	1.62%	0.190%
34	13.953	2034	2040	2043	rBV2	35910	62309	4.07%	0.477%
35	13.994	2043	2047	2061	rVB2	125779	283031	18.49%	2.166%
36	14.117	2063	2068	2074	rVB5	12291	20541	1.34%	0.157%

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ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
597-A-J

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_N\methods\82N121223W.M
Title : SW846 8260

37	14.182	2074	2079	2084	rBV3	12705	19738	1.29%	0.151%
38	14.241	2084	2089	2093	rBV3	17559	30847	2.01%	0.236%
39	14.329	2099	2104	2111	rVB	59864	92388	6.03%	0.707%
40	14.400	2111	2116	2118	rBV2	19165	28008	1.83%	0.214%
41	14.447	2118	2124	2133	rVB2	112978	202195	13.21%	1.548%
42	14.576	2140	2146	2152	rVB5	17332	35539	2.32%	0.272%
43	14.653	2152	2159	2163	rBV	28995	52827	3.45%	0.404%
44	14.688	2163	2165	2170	rVV3	12833	20014	1.31%	0.153%
45	14.929	2201	2206	2213	rBV2	31560	59242	3.87%	0.453%
46	15.053	2218	2227	2235	rBV3	81284	198119	12.94%	1.516%
47	15.211	2249	2254	2260	rBV5	14823	26066	1.70%	0.200%
48	15.317	2266	2272	2277	rBV6	15493	32655	2.13%	0.250%
49	15.441	2287	2293	2300	rVB6	19293	42662	2.79%	0.327%
50	15.641	2320	2327	2334	rVB	41006	76574	5.00%	0.586%
51	16.782	2513	2521	2522	rBV2	31359	50410	3.29%	0.386%

Sum of corrected areas: 13065142

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ClientSampleId :
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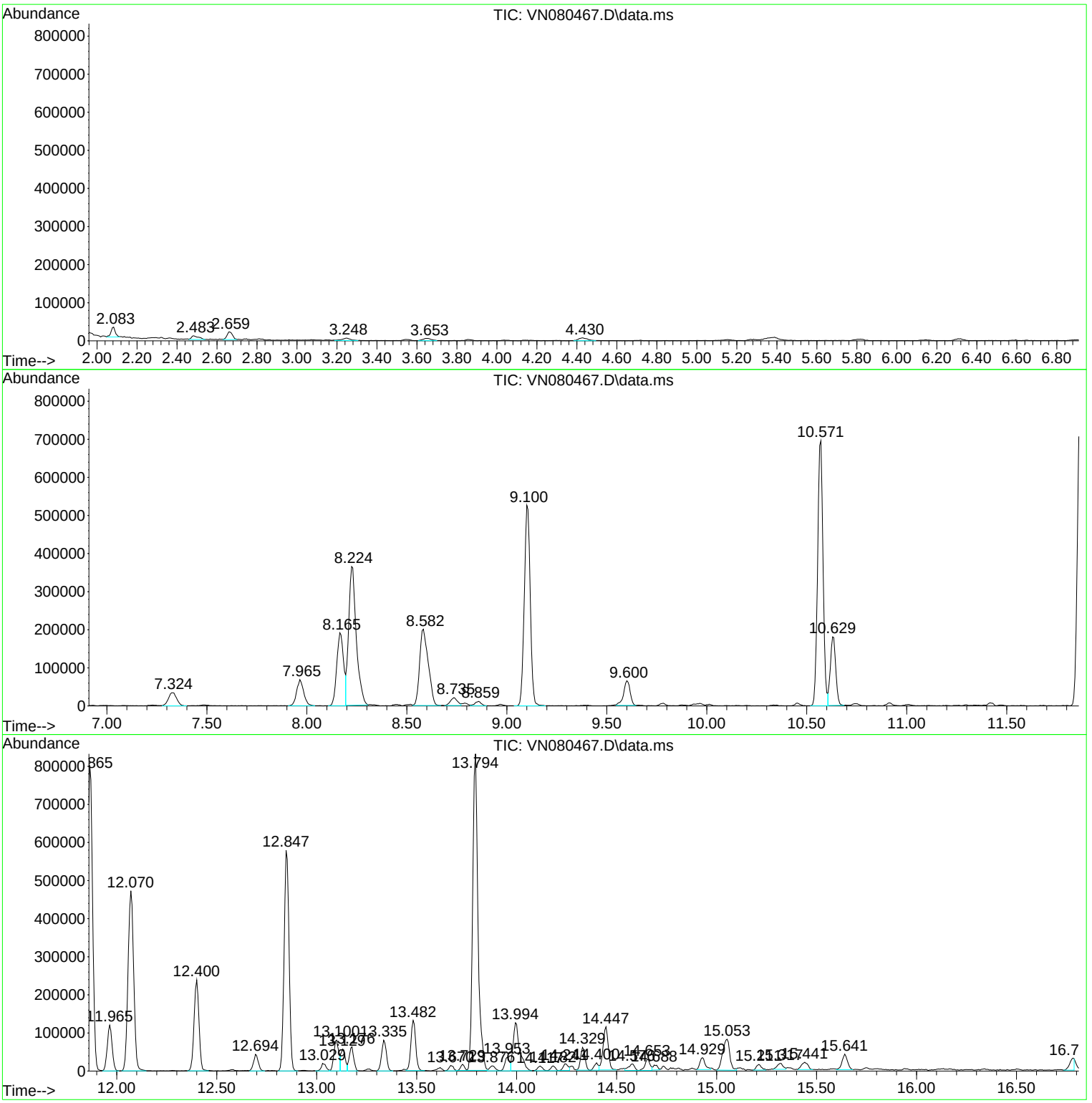
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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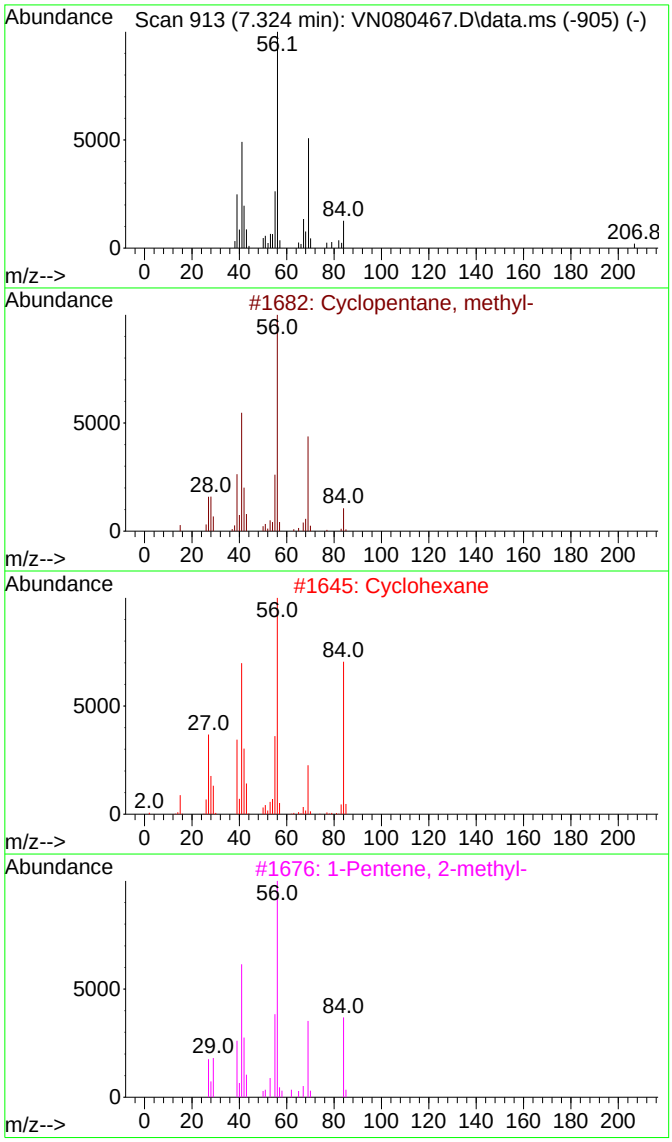
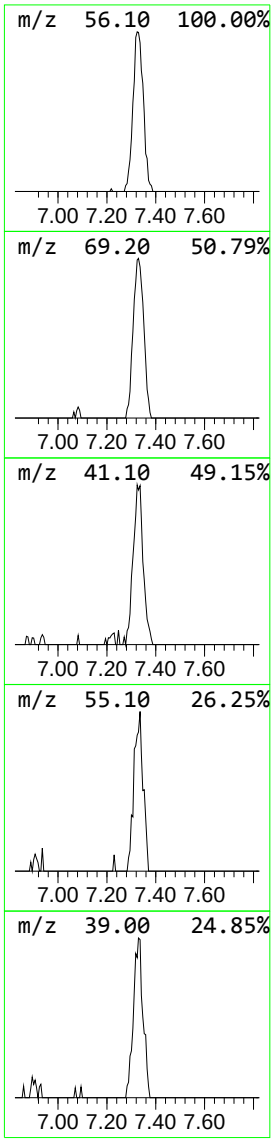
****
Peak Number 1 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.324	5.19 ug/l	98998	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclohexane	84	C6H12	000110-82-7	72
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
4	1-Heptene, 6-methyl-	112	C8H16	005026-76-6	56
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	53





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

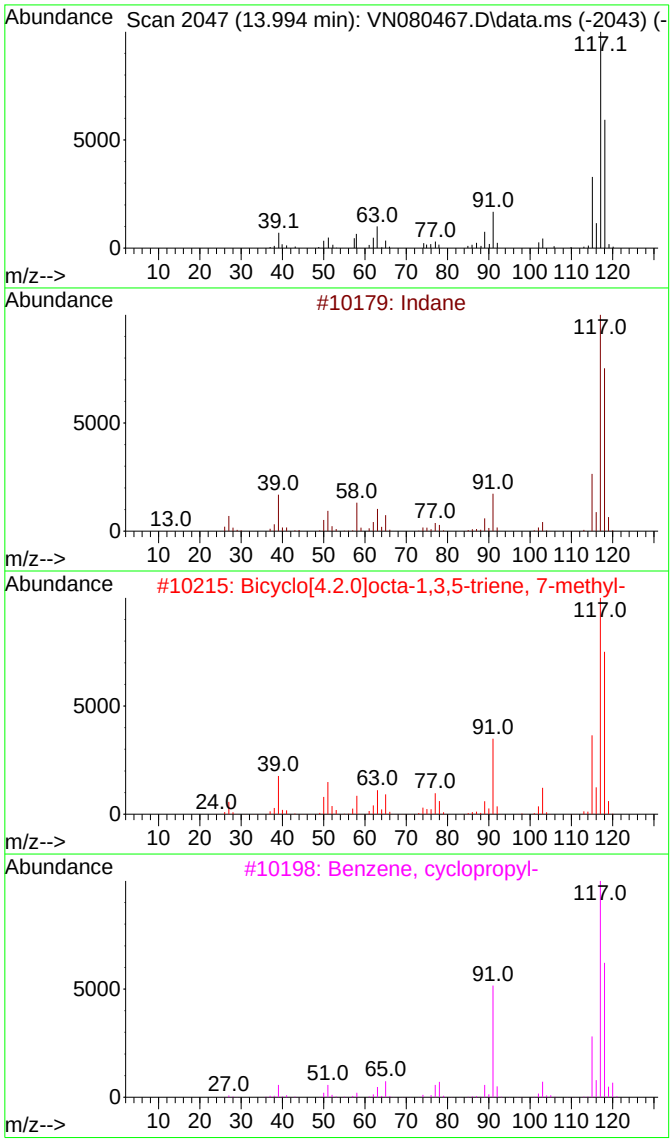
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

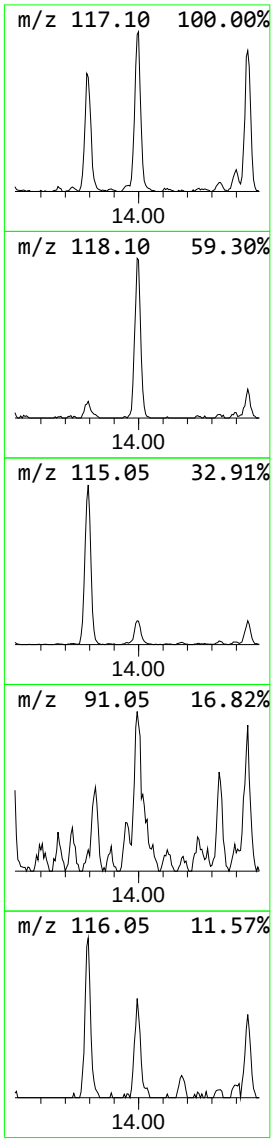
****

Peak Number 2 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	9.24 ug/l	283031	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	87
2	Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	72
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	72
4	3-Phenyl-1-propanol, acetate	178	C11H14O2	000122-72-5	59
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	59





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ClientSampleId :
597-A-J

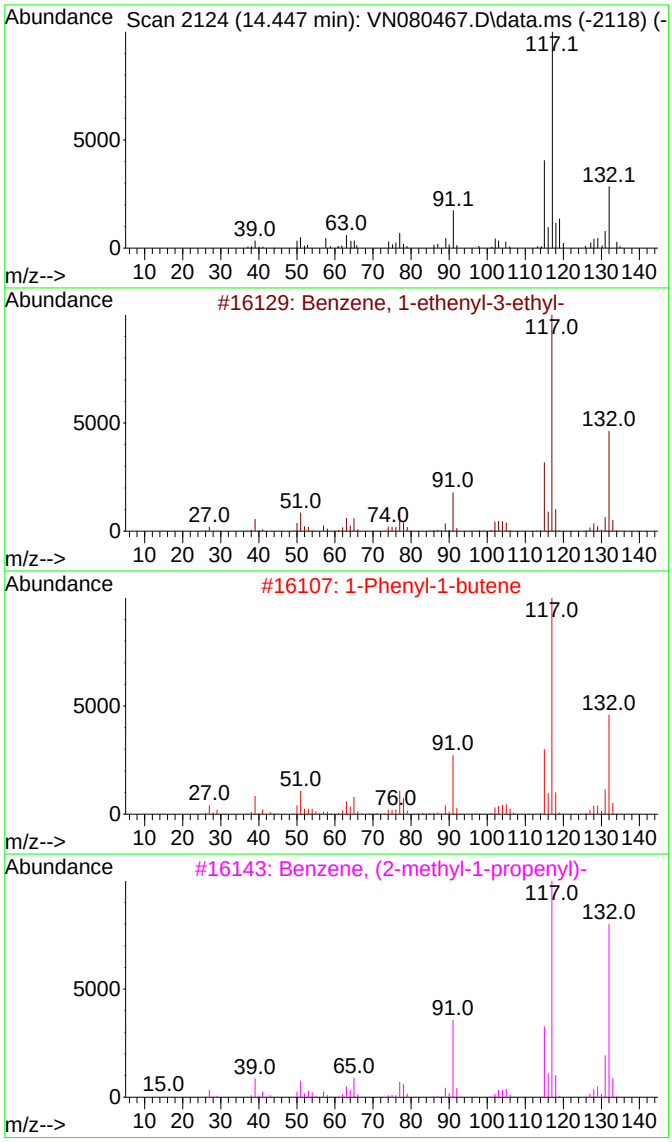
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

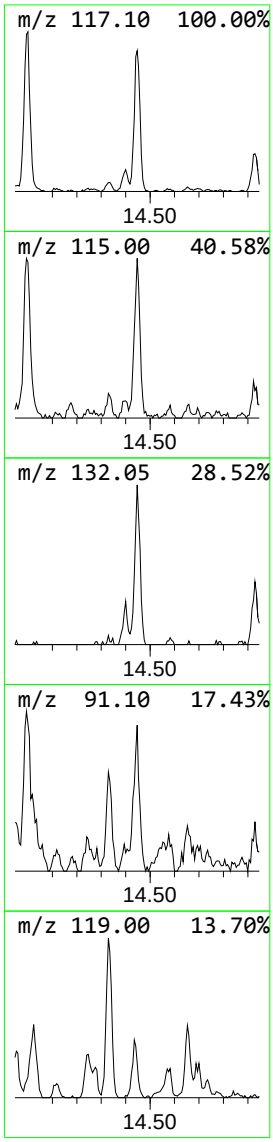
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.447	6.60 ug/l	202195	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
3	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	86
4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	80
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	80





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Instrument :
MSVOA_N
ClientSampleId :
597-A-J

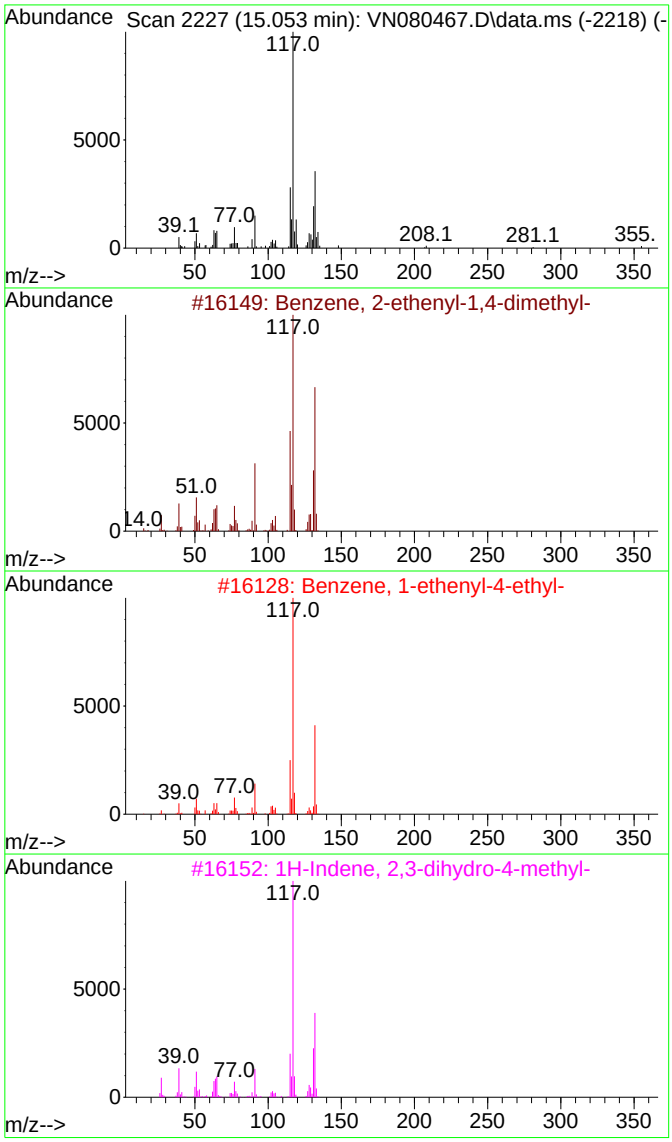
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

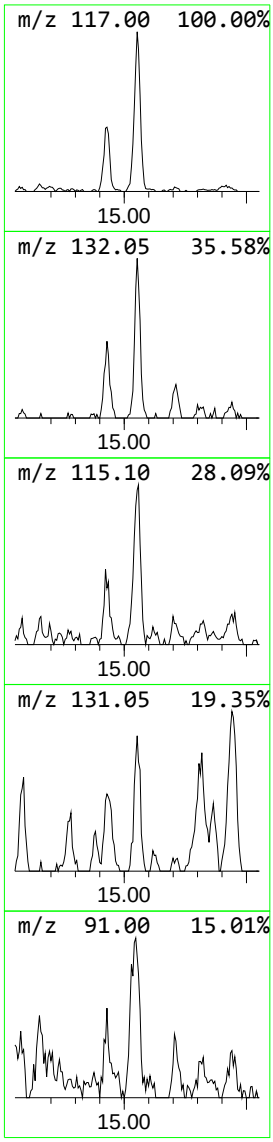
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	6.47 ug/l	198119	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	90
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	81
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	81





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclopentane, m...	7.324	5.2	ug/l	98998	1	8.230	953788	50.0
Indane	13.994	9.2	ug/l	283031	4	13.794	1530940	50.0
Benzene, 1-ethe...	14.447	6.6	ug/l	202195	4	13.794	1530940	50.0
Benzene, 2-ethe...	15.053	6.5	ug/l	198119	4	13.794	1530940	50.0