LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112222\
Data File : VN075375.D
Acq On : 22 Nov 2022 18:07
Operator : JC\MD
Sample : N5644-01
Misc : 1.03g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
102122

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\82N112122W.M
Title : SW846 8260

Signal : TIC: VN075375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.295	35	41	52	rVB4	10191	27660	2.25%	0.420%
2	3.118	180	181	190	rVB7	22283	35989	2.93%	0.547%
3	5.495	575	585	595	rBV3	4774	15306	1.25%	0.233%
4	8.171	1030	1040	1043	rBV	72853	170073	13.85%	2.584%
5	8.224	1043	1049	1059	rVB	212140	476962	38.85%	7.246%
6	8.441	1079	1086	1092	rBB4	6005	12974	1.06%	0.197%
7	8.577	1102	1109	1120	rBV	56902	126217	10.28%	1.917%
8	8.706	1124	1131	1132	rBV2	20437	38969	3.17%	0.592%
9	9.100	1189	1198	1212	rVB	297865	601928	49.03%	9.145%
10	10.012	1346	1353	1362	rVB4	5449	13215	1.08%	0.201%
11	10.141	1371	1375	1382	rBV5	7750	15449	1.26%	0.235%
12	10.341	1402	1409	1414	rBV2	6981	13946	1.14%	0.212%
13	10.565	1440	1447	1452	rBV	173898	319219	26.00%	4.850%
14	10.630	1452	1458	1467	rVV	682774	1227700	100.00%	18.651%
15	10.747	1471	1478	1484	rVB5	10985	23060	1.88%	0.350%
16	11.647	1622	1631	1636	rBV3	13836	27175	2.21%	0.413%
17	11.747	1642	1648	1652	rBV2	13594	21088	1.72%	0.320%
18	11.865	1659	1668	1678	rBV	378206	685017	55.80%	10.407%
19	11.965	1678	1685	1691	rVB2	21193	36661	2.99%	0.557%
20	12.071	1691	1703	1712	rBV3	58801	120133	9.79%	1.825%
21	12.400	1754	1759	1768	rVB2	13220	25708	2.09%	0.391%
22	12.700	1805	1810	1814	rBV2	9514	16943	1.38%	0.257%
23	12.853	1829	1836	1846	rVB	241527	446414	36.36%	6.782%
24	13.035	1862	1867	1873	rBV	38435	59617	4.86%	0.906%
25	13.100	1873	1878	1881	rVV	33802	55455	4.52%	0.842%
26	13.135	1881	1884	1887	rVV	34684	58874	4.80%	0.894%
27	13.171	1887	1890	1897	rVB2	37409	64586	5.26%	0.981%
28	13.335	1909	1918	1925	rBV	25577	49983	4.07%	0.759%
29	13.482	1937	1943	1950	rBV	101745	162061	13.20%	2.462%
30	13.729	1980	1985	1988	rVV4	6771	14410	1.17%	0.219%
31	13.794	1989	1996	2013	rVB	394081	705336	57.45%	10.716%
32	13.953	2016	2023	2025	rBV2	22509	34981	2.85%	0.531%
33	13.994	2025	2030	2032	rVV3	43829	84855	6.91%	1.289%
34	14.029	2032	2036	2045	rVV3	46556	122760	10.00%	1.865%
35	14.106	2045	2049	2055	rVB4	7105	12524	1.02%	0.190%
36	14.188	2057	2063	2067	rVB	14853	23161	1.89%	0.352%

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Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Title : SW846 8260

37	14.247	2067	2073	2075	rBV	18906	28140	2.29%	0.428%
38	14.276	2075	2078	2082	rVV2	17313	24816	2.02%	0.377%
39	14.329	2082	2087	2093	rVV	63182	99333	8.09%	1.509%
40	14.447	2101	2107	2113	rVB2	30899	53614	4.37%	0.815%
41	14.582	2123	2130	2134	rBV4	9659	19962	1.63%	0.303%
42	14.653	2134	2142	2146	rVV	27062	53866	4.39%	0.818%
43	14.694	2146	2149	2152	rVV	20439	29804	2.43%	0.453%
44	14.735	2152	2156	2160	rVV2	19928	30836	2.51%	0.468%
45	14.876	2177	2180	2184	rVB3	10053	13212	1.08%	0.201%
46	14.935	2184	2190	2194	rBV3	35102	76832	6.26%	1.167%
47	15.053	2200	2210	2215	rBV5	36970	97141	7.91%	1.476%
48	15.094	2215	2217	2223	rVB2	12157	19727	1.61%	0.300%
49	15.323	2251	2256	2260	rVV3	15446	26610	2.17%	0.404%
50	15.441	2268	2276	2284	rBV8	12308	29586	2.41%	0.449%
51	15.641	2304	2310	2315	rVB3	11604	19989	1.63%	0.304%
52	15.835	2335	2343	2348	rVB7	4789	12496	1.02%	0.190%

Sum of corrected areas: 6582373

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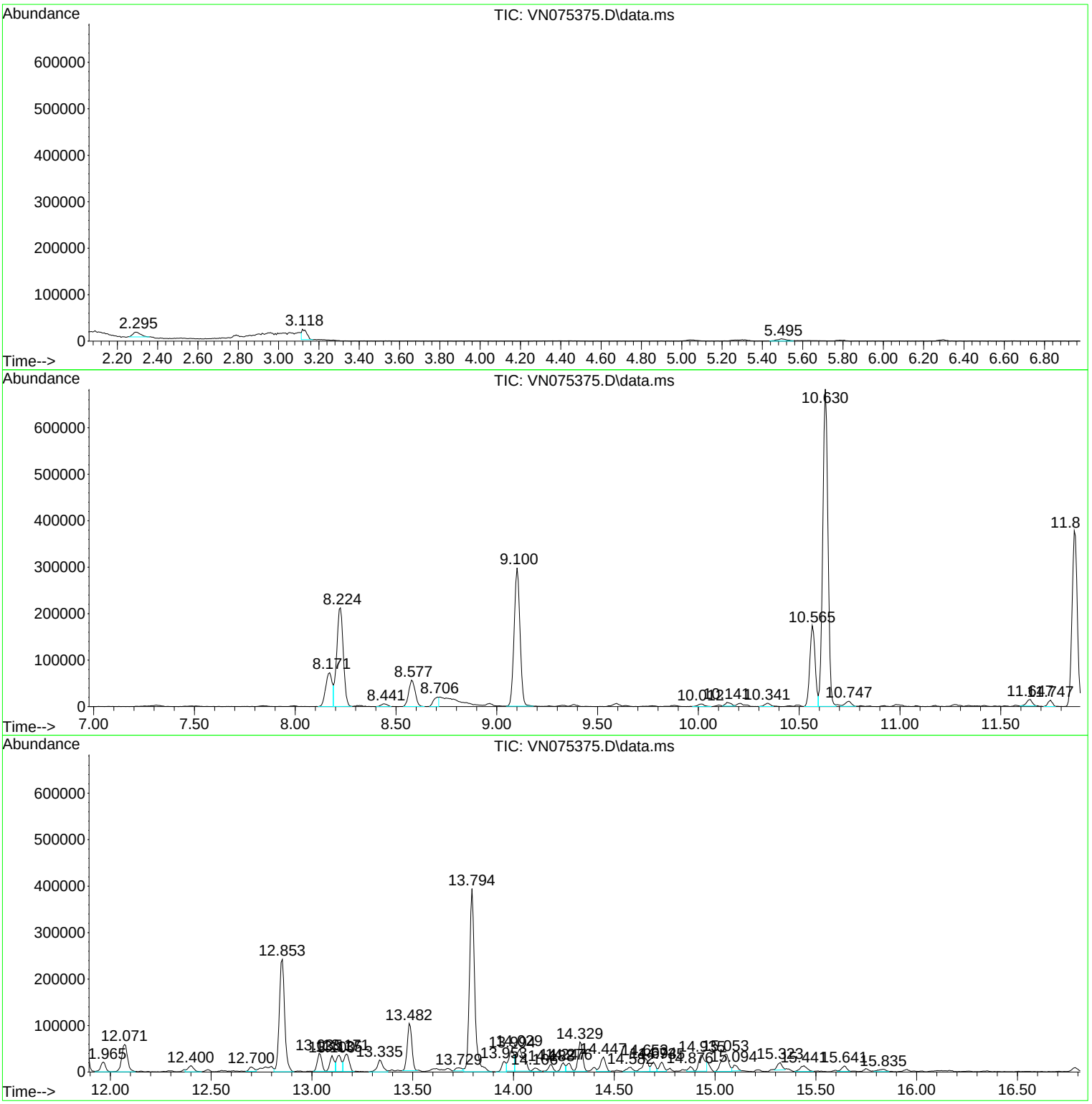
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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



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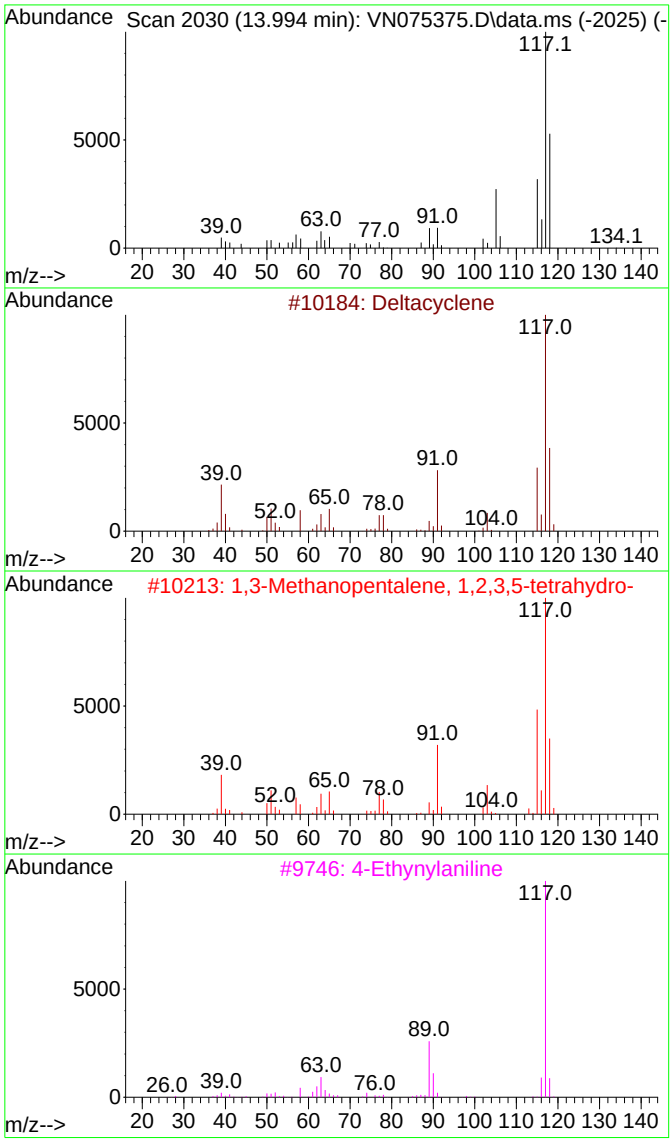
Quant Title : SW846 8260

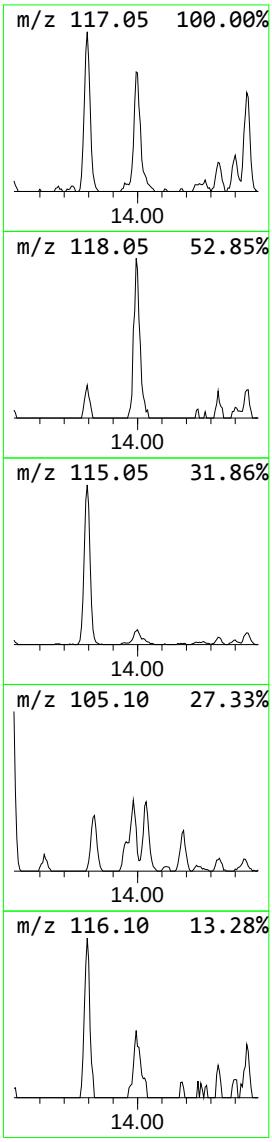
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1,3-Methanopentalene, 1,2,3... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	6.02 ug/l	84855	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	53
2	1,3-Methanopentalene, 1,2,3,5-te...	118	C9H10	128600-88-4	53
3	4-Ethynylaniline	117	C8H7N	014235-81-5	43
4	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	40
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	38





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Instrument :
MSVOA_N
ClientSampleId :
102122

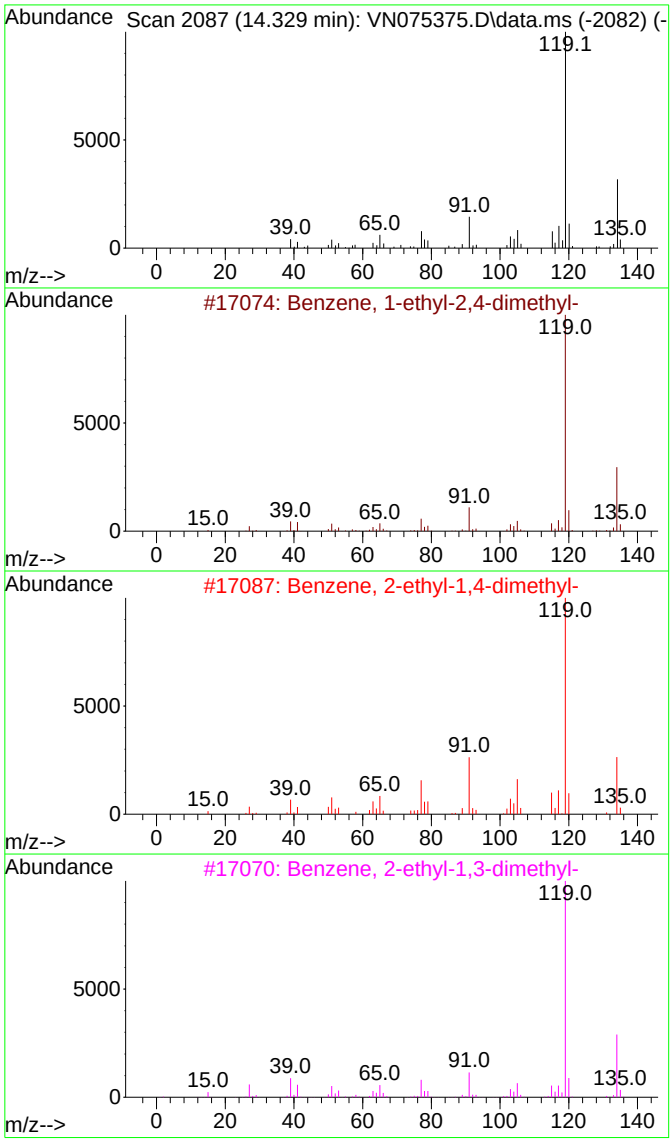
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

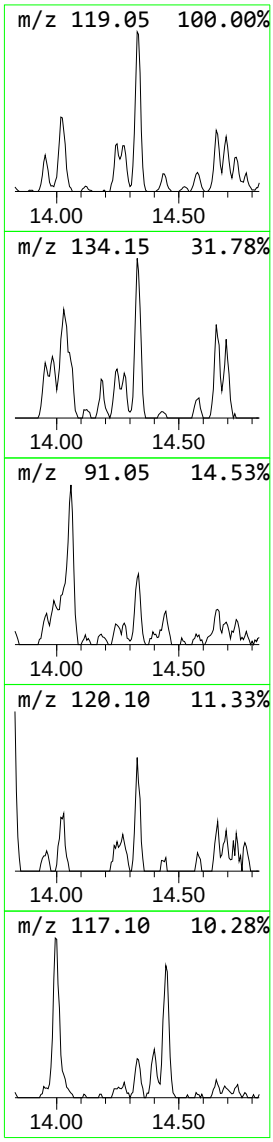
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.329	7.04 ug/l	99333	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	96
3	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
5	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94





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Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

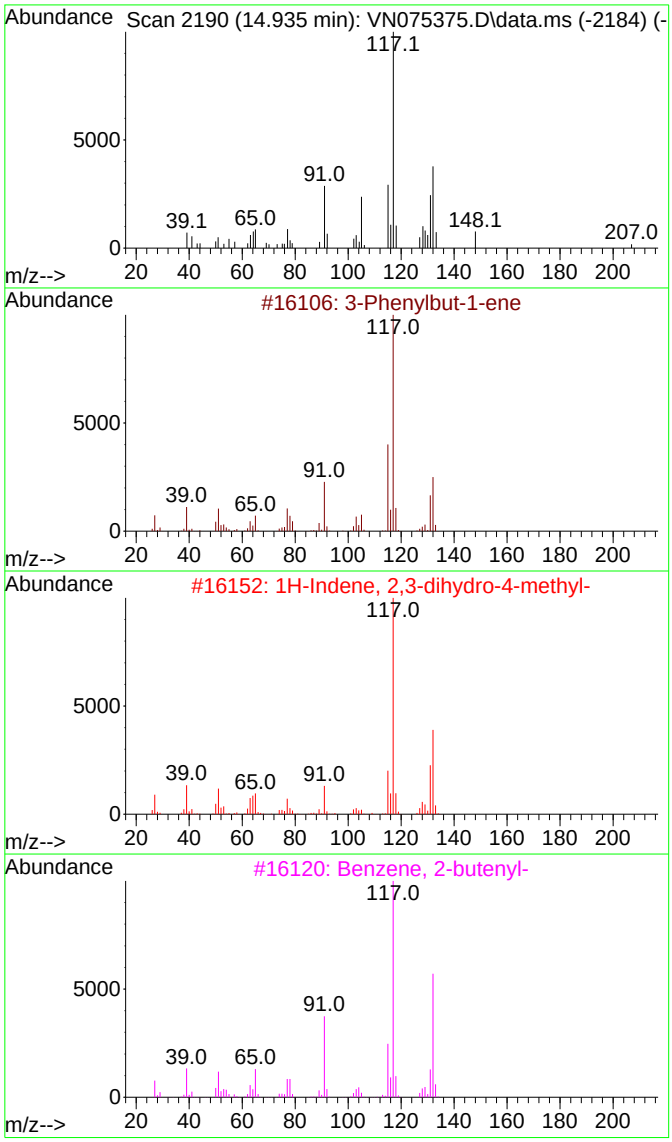
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

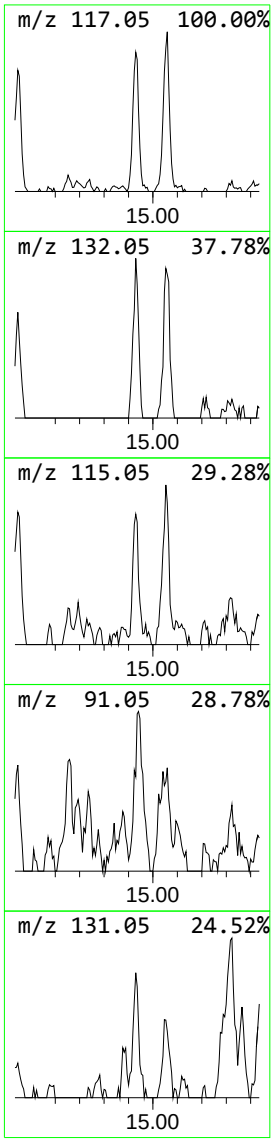
****

Peak Number 3 3-Phenylbut-1-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.935	5.45 ug/l	76832	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	83
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	81
3	Benzene, 2-butenyl-	132	C10H12	001560-06-1	76
4	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76
5	Azulene, 1,2,3,3a-tetrahydro-	132	C10H12	033877-87-1	74





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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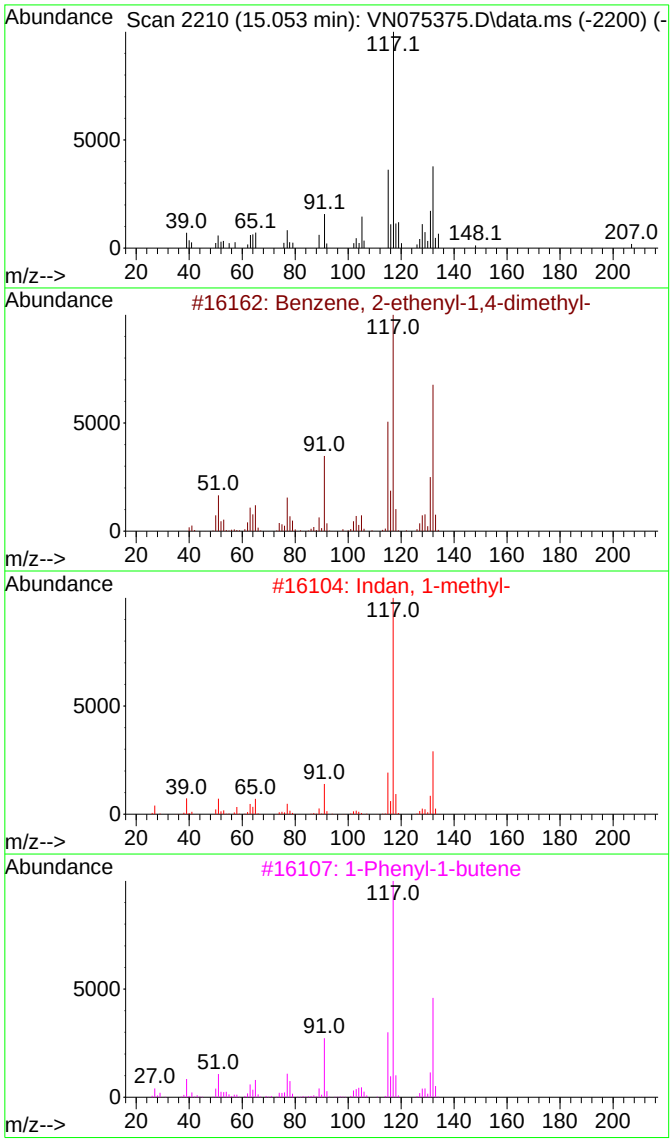
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

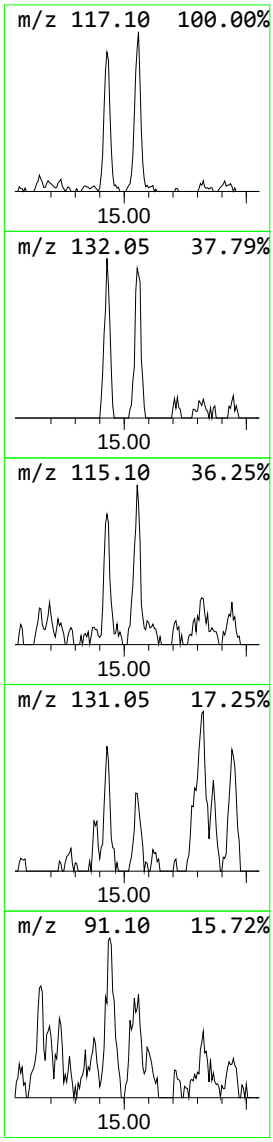
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	6.89 ug/l	97141	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	90
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1,3-Methanopent...	13.994	6.0	ug/l	84855	4	13.794	705336	50.0
Benzene, 1-ethy...	14.329	7.0	ug/l	99333	4	13.794	705336	50.0
3-Phenylbut-1-ene	14.935	5.5	ug/l	76832	4	13.794	705336	50.0
Benzene, 2-ethe...	15.053	6.9	ug/l	97141	4	13.794	705336	50.0