LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN111924\
Data File : VN084941.D
Acq On : 19 Nov 2024 12:52
Operator : JC\MD
Sample : P4770-02 500X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-3

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\82N103024W.M
Title : SW846 8260

Signal : TIC: VN084941.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	50	58	67	rBV3	20168	47318	3.68%	0.408%
2	2.871	143	156	158	rBV7	11800	32567	2.53%	0.281%
3	7.224	885	896	902	rBV4	6590	19431	1.51%	0.168%
4	7.312	905	911	921	rVB5	5531	14319	1.11%	0.124%
5	8.165	1044	1056	1060	rBV	154847	370769	28.81%	3.198%
6	8.218	1060	1065	1077	rVV	286123	640327	49.75%	5.523%
7	8.324	1077	1083	1090	rVB4	7521	18986	1.48%	0.164%
8	8.441	1096	1103	1110	rVB2	10501	22841	1.77%	0.197%
9	8.577	1116	1126	1136	rBV	167398	397449	30.88%	3.428%
10	8.753	1142	1156	1171	rBV3	38100	134137	10.42%	1.157%
11	8.965	1186	1192	1203	rVB3	6445	15137	1.18%	0.131%
12	9.100	1206	1215	1223	rBV	404360	836561	64.99%	7.216%
13	9.588	1289	1298	1303	rBV5	12131	29118	2.26%	0.251%
14	10.012	1364	1370	1379	rVB2	21219	42236	3.28%	0.364%
15	10.147	1385	1393	1399	rBV2	31365	62952	4.89%	0.543%
16	10.335	1416	1425	1439	rBV5	5919	17985	1.40%	0.155%
17	10.488	1447	1451	1456	rVB2	9794	16482	1.28%	0.142%
18	10.565	1456	1464	1469	rVV	595379	1097276	85.25%	9.465%
19	10.630	1469	1475	1488	rVV	689316	1287159	100.00%	11.103%
20	11.865	1676	1685	1695	rBV	544147	962885	74.81%	8.306%
21	11.959	1695	1701	1709	rVV	179145	304030	23.62%	2.622%
22	12.065	1711	1719	1730	rVV	490185	935695	72.69%	8.071%
23	12.394	1767	1775	1784	rBV	194437	331606	25.76%	2.860%
24	12.694	1820	1826	1835	rVB	50796	81110	6.30%	0.700%
25	12.847	1841	1852	1863	rVB	474293	776520	60.33%	6.698%
26	13.035	1878	1884	1889	rBV2	62913	102108	7.93%	0.881%
27	13.094	1889	1894	1898	rVV	173129	297669	23.13%	2.568%
28	13.129	1898	1900	1903	rVV	87566	107447	8.35%	0.927%
29	13.171	1903	1907	1914	rVB	98474	163160	12.68%	1.407%
30	13.335	1928	1935	1941	rVB	69123	112347	8.73%	0.969%
31	13.482	1953	1960	1967	rVB	334629	535312	41.59%	4.617%
32	13.612	1975	1982	1987	rBV3	7251	19733	1.53%	0.170%
33	13.788	2005	2012	2026	rVB2	539940	1061271	82.45%	9.154%
34	13.988	2033	2046	2049	rBV2	73225	169502	13.17%	1.462%
35	14.176	2074	2078	2084	rVB4	13364	21499	1.67%	0.185%
36	14.241	2084	2089	2092	rBV	25515	41188	3.20%	0.355%

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Integration Parameters: RTEINT.P
Integrator: RTE
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Title : SW846 8260

37	14.270	2092	2094	2099	rVV2	22703	30545	2.37%	0.263%
38	14.329	2099	2104	2109	rVB	44339	67387	5.24%	0.581%
39	14.441	2118	2123	2129	rVB3	14132	25451	1.98%	0.220%
40	14.570	2138	2145	2151	rBV4	10149	17006	1.32%	0.147%
41	14.653	2151	2159	2162	rBV	25984	44088	3.43%	0.380%
42	14.694	2162	2166	2170	rVV	36801	58590	4.55%	0.505%
43	14.923	2201	2205	2209	rBV2	15992	25561	1.99%	0.220%
44	15.047	2216	2226	2234	rBV6	30010	84297	6.55%	0.727%
45	15.317	2267	2272	2280	rBV5	7823	18216	1.42%	0.157%
46	15.641	2320	2327	2334	rVB	37875	74559	5.79%	0.643%
47	16.776	2512	2520	2522	rBV	12693	21325	1.66%	0.184%

Sum of corrected areas: 11593157

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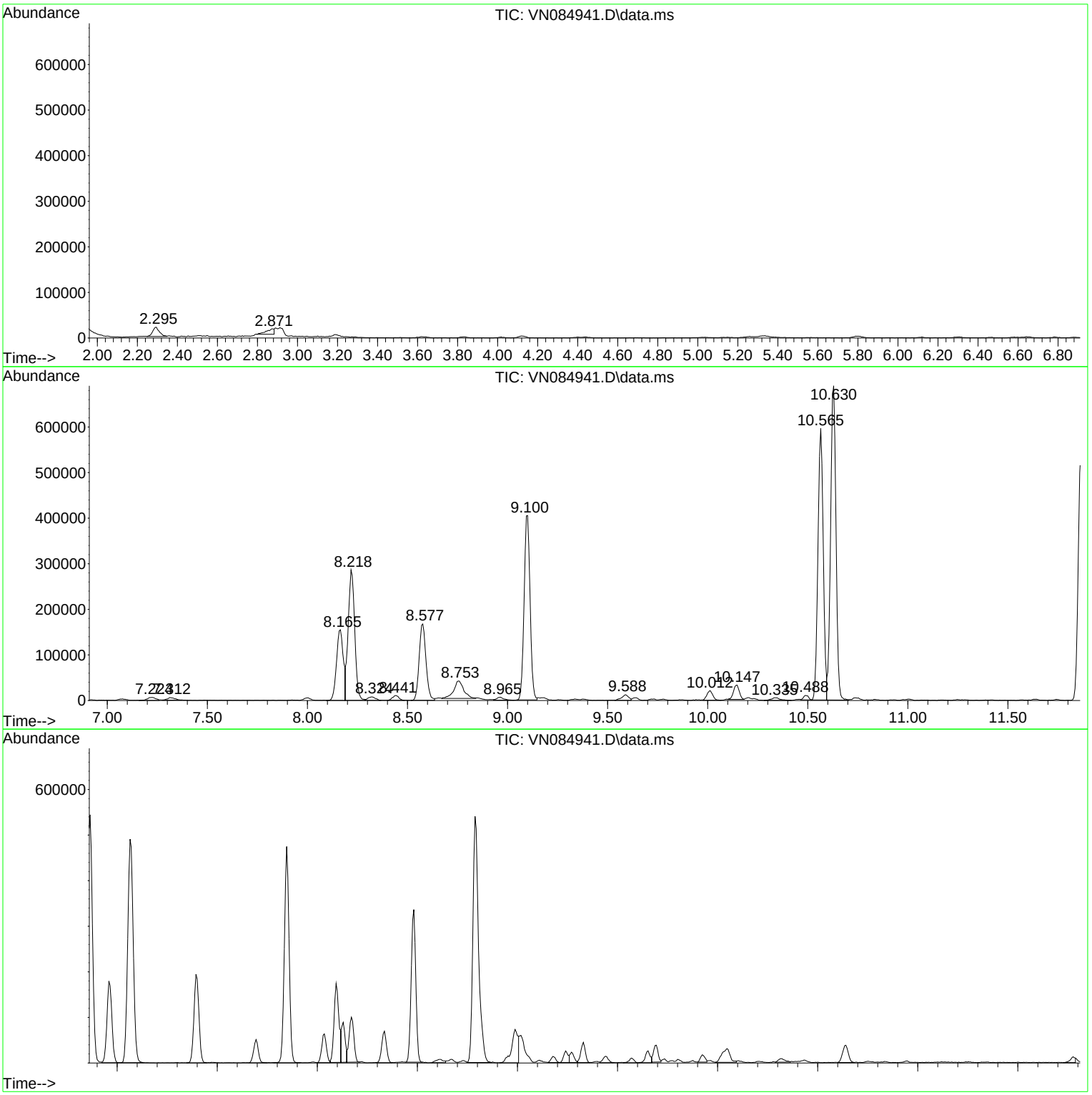
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

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



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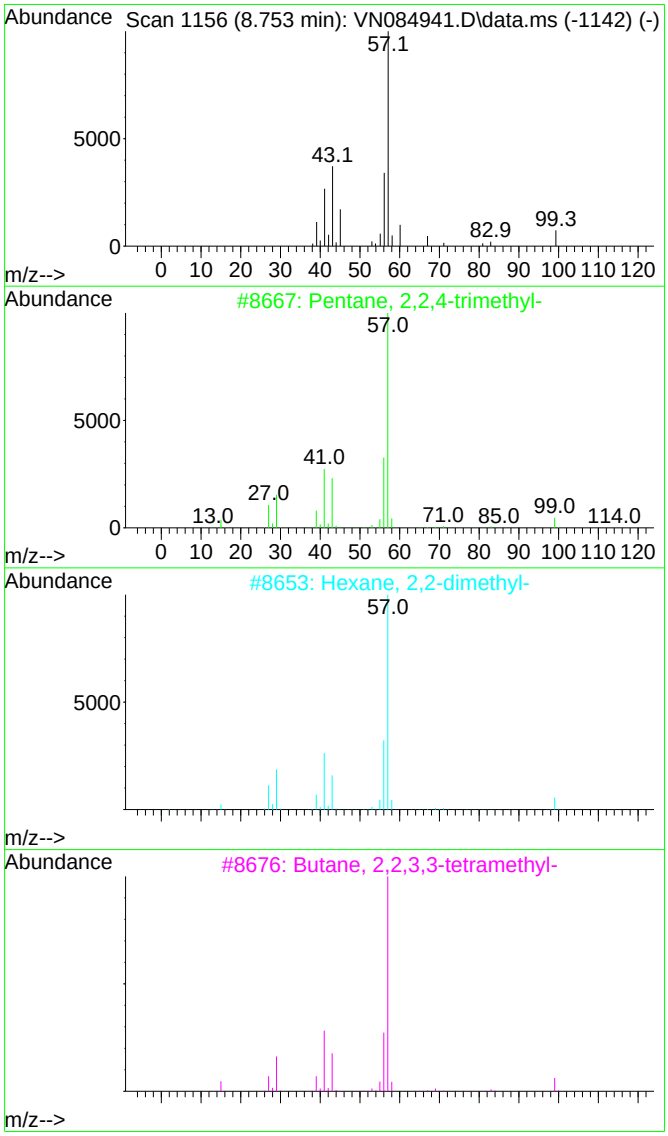
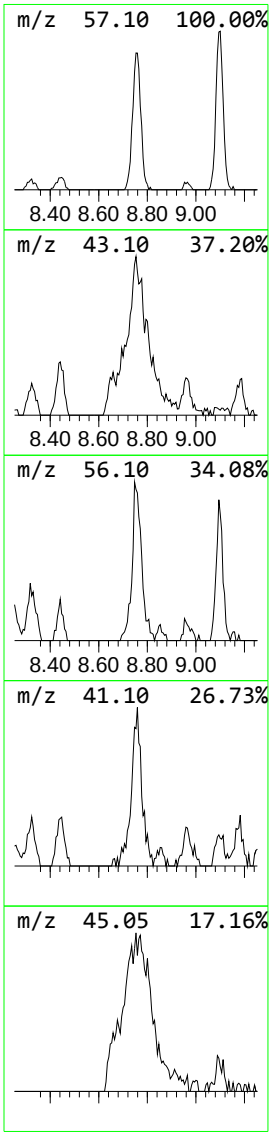
****
Peak Number 1 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.753	8.02 ug/l	134137	1,4-Difluorobenzene	9.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	50
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	40
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
4	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	38
5	Octane, 3-methyl-	128	C9H20	002216-33-3	37





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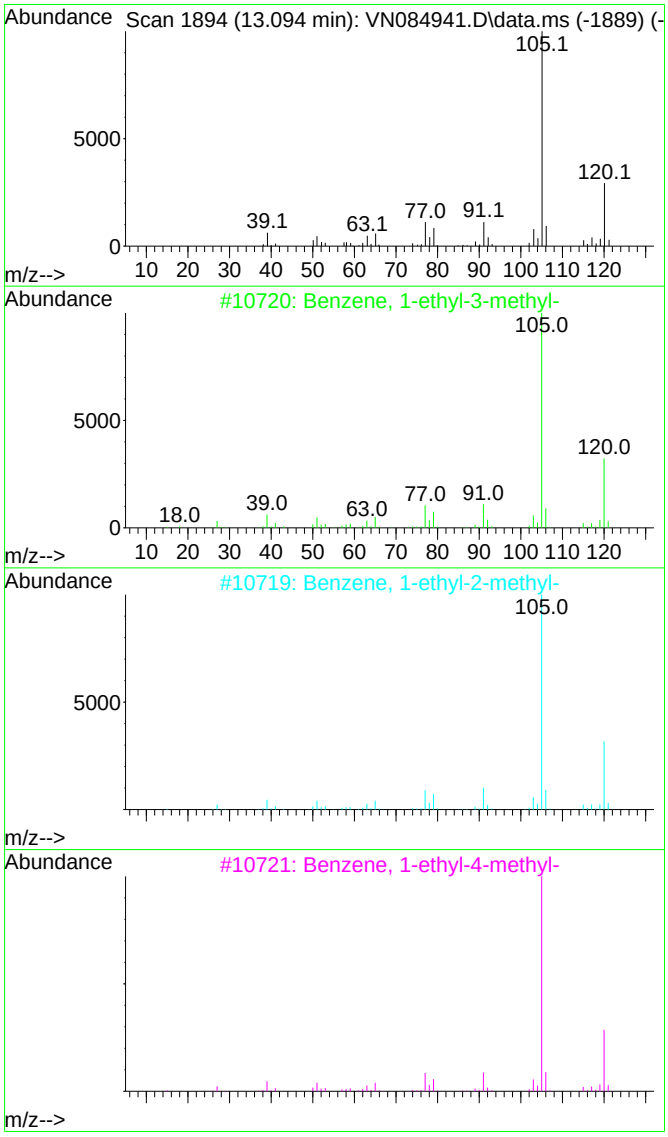
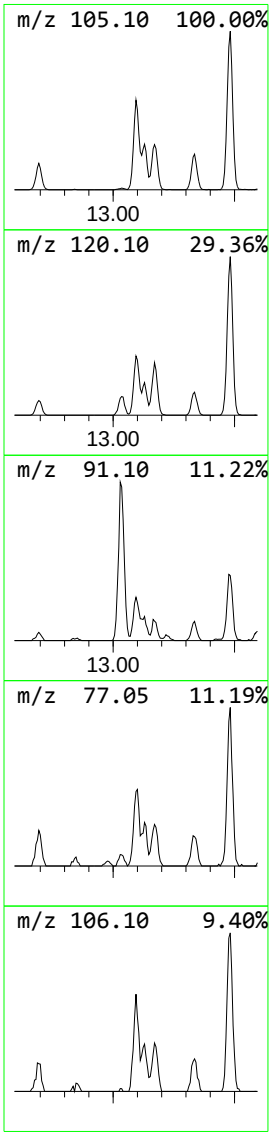
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.094	14.02 ug/l	297669	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90





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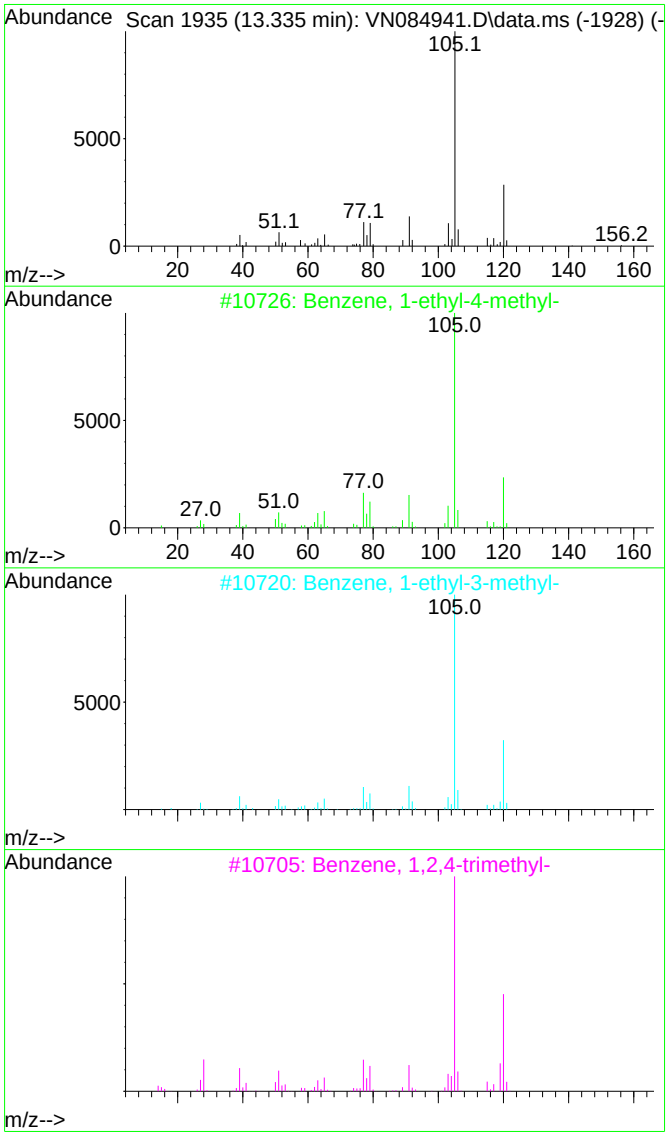
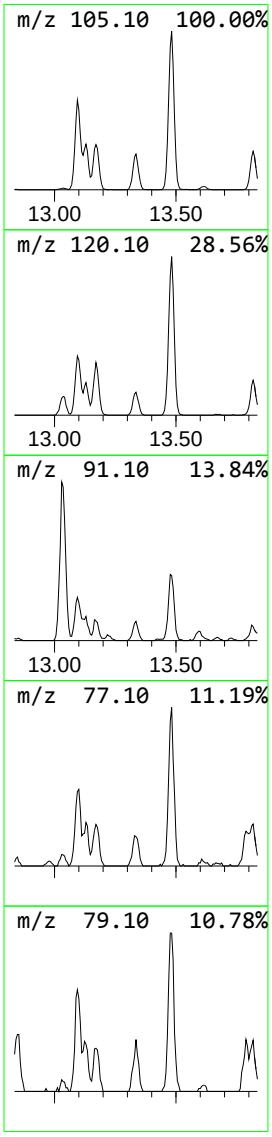
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	5.29 ug/l	112347	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91





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Instrument :
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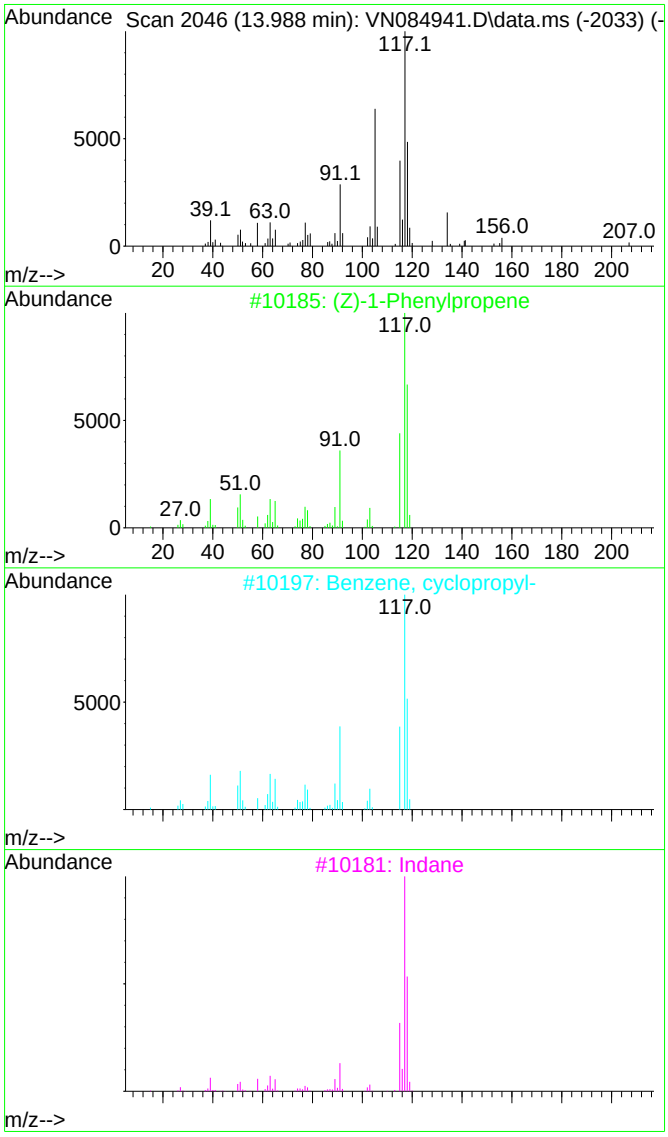
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N103024W.M
Quant Title : SW846 8260

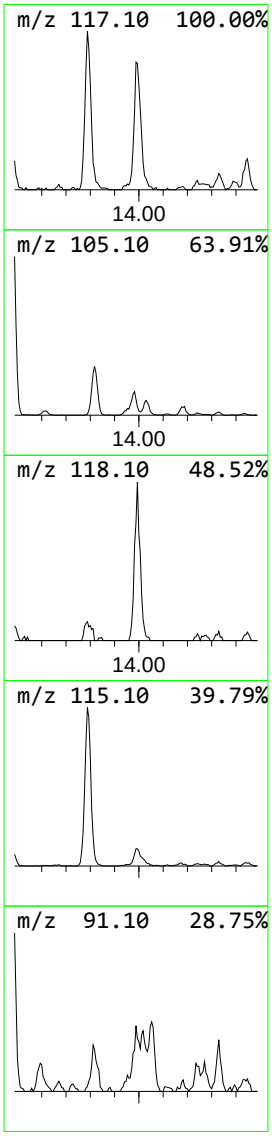
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (Z)-1-Phenylpropene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.988	7.99 ug/l	169502	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	78
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60
3	Indane	118	C9H10	000496-11-7	60
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	58
5	Deltacyclene	118	C9H10	007785-10-6	58





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 2,2,4-...	8.753	8.0	ug/l	134137	2	9.094	836561	50.0
Benzene, 1-ethy...	13.094	14.0	ug/l	297669	4	13.788	1061270	50.0
Benzene, 1-ethy...	13.335	5.3	ug/l	112347	4	13.788	1061270	50.0
(Z)-1-Phenylpro...	13.988	8.0	ug/l	169502	4	13.788	1061270	50.0