LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_U\Method\SFAMULM052924WMA.M
Title : VOC Analysis

Signal : TIC: VU059390.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	55	58	64	rVB2	1780	1886	0.25%	0.033%
2	1.592	86	94	116	rBV	53149	87224	11.35%	1.514%
3	1.846	136	173	176	rBV6	56760	236826	30.83%	4.110%
4	2.537	376	388	407	rBV	131042	214475	27.92%	3.723%
5	2.631	409	417	434	rVB2	4001	7816	1.02%	0.136%
6	2.769	449	460	461	rBV2	1134	1280	0.17%	0.022%
7	2.946	505	515	530	rBV	7588	15439	2.01%	0.268%
8	3.029	531	541	554	rVV2	5837	10139	1.32%	0.176%
9	3.174	583	586	593	rVB3	503	583	0.08%	0.010%
10	3.293	619	623	631	rVV2	227	286	0.04%	0.005%
11	3.804	773	782	784	rBV2	204	288	0.04%	0.005%
12	4.081	865	868	875	rVB2	338	319	0.04%	0.006%
13	4.132	879	884	891	rBV2	293	364	0.05%	0.006%
14	4.621	1025	1036	1062	rBV	82913	228947	29.80%	3.974%
15	5.052	1154	1170	1200	rVV	138731	308906	40.21%	5.362%
16	5.206	1216	1218	1222	rVB	379	243	0.03%	0.004%
17	5.515	1310	1314	1319	rVB	271	317	0.04%	0.006%
18	5.711	1356	1375	1401	rBV2	282971	768262	100.00%	13.334%
19	6.045	1475	1479	1486	rVB2	235	300	0.04%	0.005%
20	6.242	1527	1540	1560	rBV	102129	195291	25.42%	3.390%
21	6.377	1580	1582	1588	rVB2	297	342	0.04%	0.006%
22	6.418	1588	1595	1597	rVB3	316	326	0.04%	0.006%
23	6.473	1606	1612	1616	rBV2	219	304	0.04%	0.005%
24	6.524	1616	1628	1640	rBV5	4699	9414	1.23%	0.163%
25	6.614	1654	1656	1661	rVB2	443	360	0.05%	0.006%
26	6.682	1661	1677	1696	rBV	179961	352450	45.88%	6.117%
27	7.193	1829	1836	1848	rBV5	2797	4927	0.64%	0.086%
28	7.248	1850	1853	1856	rVV3	499	315	0.04%	0.005%
29	7.560	1939	1950	1974	rVV	87123	158967	20.69%	2.759%
30	7.701	1986	1994	1996	rBV3	1322	1745	0.23%	0.030%
31	7.891	2040	2053	2071	rBV	330399	583298	75.92%	10.124%
32	8.174	2129	2141	2162	rBV	59522	106724	13.89%	1.852%
33	8.254	2162	2166	2169	rBV2	274	254	0.03%	0.004%
34	8.460	2226	2230	2231	rBV	432	307	0.04%	0.005%
35	8.550	2250	2258	2264	rVV6	829	1070	0.14%	0.019%
36	8.637	2272	2285	2323	rBV	242224	520210	67.71%	9.029%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_U\Method\SFAMULM052924WMA.M
Title : VOC Analysis

37	9.277	2477	2484	2488	rBV	255	329	0.04%	0.006%
38	9.335	2499	2502	2506	rVB	369	263	0.03%	0.005%
39	9.357	2506	2509	2511	rBV	334	270	0.04%	0.005%
40	9.415	2516	2527	2546	rBV	146337	253335	32.98%	4.397%
41	9.573	2568	2576	2579	rBV4	764	1110	0.14%	0.019%
42	9.692	2609	2613	2615	rVV	570	507	0.07%	0.009%
43	9.708	2615	2618	2626	rVV2	1008	988	0.13%	0.017%
44	10.074	2727	2732	2736	rBV2	303	291	0.04%	0.005%
45	10.142	2750	2753	2758	rVB2	273	294	0.04%	0.005%
46	10.171	2758	2762	2767	rBV2	342	393	0.05%	0.007%
47	10.203	2767	2772	2776	rVV	311	305	0.04%	0.005%
48	10.257	2787	2789	2793	rVV2	241	232	0.03%	0.004%
49	10.290	2797	2799	2807	rVB2	253	262	0.03%	0.005%
50	10.666	2912	2916	2925	rVB4	749	1028	0.13%	0.018%
51	10.753	2931	2943	2967	rBV	315483	525895	68.45%	9.128%
52	10.884	2978	2984	2986	rBV3	400	387	0.05%	0.007%
53	11.100	3047	3051	3055	rVB3	324	249	0.03%	0.004%
54	11.341	3120	3126	3131	rBV2	176	244	0.03%	0.004%
55	11.447	3156	3159	3161	rBV	448	232	0.03%	0.004%
56	11.473	3164	3167	3168	rBV2	444	233	0.03%	0.004%
57	11.695	3224	3236	3245	rBV6	4601	7117	0.93%	0.124%
58	11.810	3260	3272	3292	rBV	160812	266207	34.65%	4.620%
59	11.939	3304	3312	3317	rBV6	3634	6010	0.78%	0.104%
60	12.058	3345	3349	3351	rBV3	406	302	0.04%	0.005%
61	12.074	3351	3354	3357	rVB2	355	248	0.03%	0.004%
62	12.100	3359	3362	3366	rBV3	368	311	0.04%	0.005%
63	12.122	3366	3369	3372	rBV3	873	535	0.07%	0.009%
64	12.190	3373	3390	3408	rBV	378530	629201	81.90%	10.921%
65	12.380	3444	3449	3457	rBV6	1309	2170	0.28%	0.038%
66	12.508	3485	3489	3491	rBV2	353	316	0.04%	0.005%
67	12.527	3491	3495	3500	rVV5	894	889	0.12%	0.015%
68	12.556	3500	3504	3507	rVB3	1015	697	0.09%	0.012%
69	12.582	3509	3512	3514	rBV2	584	371	0.05%	0.006%
70	12.720	3552	3555	3557	rBV2	397	237	0.03%	0.004%
71	12.810	3570	3583	3584	rBV4	1447	1874	0.24%	0.033%
72	12.878	3599	3604	3606	rBV3	322	249	0.03%	0.004%
73	12.926	3612	3619	3622	rBV3	661	675	0.09%	0.012%
74	12.942	3622	3624	3625	rBV2	724	307	0.04%	0.005%
75	12.961	3626	3630	3635	rVB5	861	927	0.12%	0.016%
76	13.016	3644	3647	3650	rBV2	335	248	0.03%	0.004%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % 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_U\Method\SFAMULM052924WMA.M
Title : VOC Analysis

77	13.080	3658	3667	3674	rBV10	1267	2054	0.27%	0.036%
78	13.142	3679	3686	3697	rVB3	8941	15481	2.02%	0.269%
79	13.225	3707	3712	3714	rBV3	974	901	0.12%	0.016%
80	13.273	3723	3727	3736	rVB6	1983	2723	0.35%	0.047%
81	13.341	3736	3748	3754	rBV10	1302	2644	0.34%	0.046%
82	13.370	3754	3757	3763	rVV5	641	551	0.07%	0.010%
83	13.437	3772	3778	3780	rBV5	1206	1195	0.16%	0.021%
84	13.521	3802	3804	3807	rBV4	474	321	0.04%	0.006%
85	13.543	3807	3811	3813	rBV4	985	735	0.10%	0.013%
86	13.749	3872	3875	3878	rBV3	798	621	0.08%	0.011%
87	13.849	3898	3906	3908	rBV6	1424	1763	0.23%	0.031%
88	13.952	3934	3938	3939	rBV	694	482	0.06%	0.008%
89	13.994	3946	3951	3959	rVB7	3137	3711	0.48%	0.064%
90	14.090	3972	3981	3995	rBV	22176	44147	5.75%	0.766%
91	14.193	4006	4013	4024	rVB8	5991	10011	1.30%	0.174%
92	14.932	4241	4243	4244	rBV2	1345	523	0.07%	0.009%
93	15.222	4324	4333	4347	rBV	29214	51696	6.73%	0.897%
94	15.408	4385	4391	4404	rVB3	12208	20539	2.67%	0.356%
95	15.955	4556	4561	4575	rVB3	8731	14562	1.90%	0.253%
96	16.122	4611	4613	4614	rBV2	1169	459	0.06%	0.008%
97	16.148	4614	4621	4627	rVV3	7878	11529	1.50%	0.200%
98	16.260	4650	4656	4663	rBV3	8640	14207	1.85%	0.247%
99	16.412	4695	4703	4709	rBV4	9932	14657	1.91%	0.254%
100	17.096	4908	4916	4930	rBV5	10842	20037	2.61%	0.348%

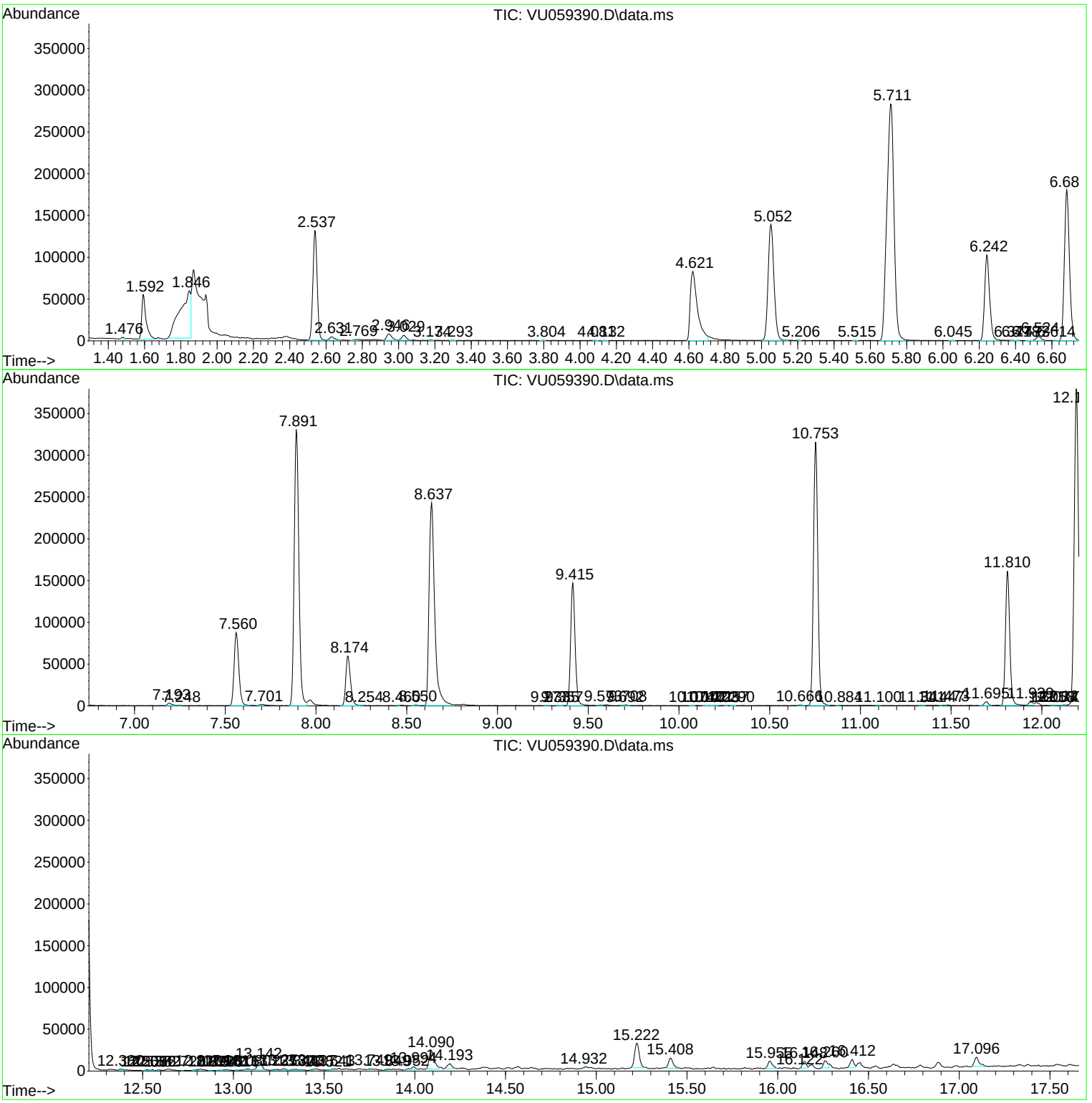
Sum of corrected areas: 5761491

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

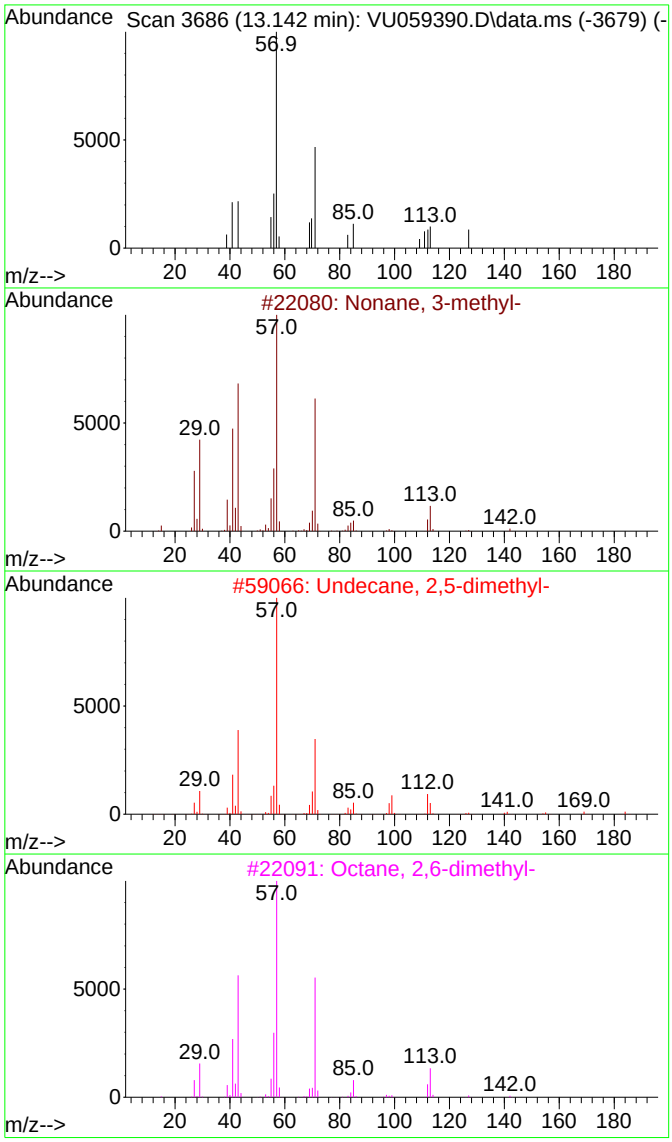
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

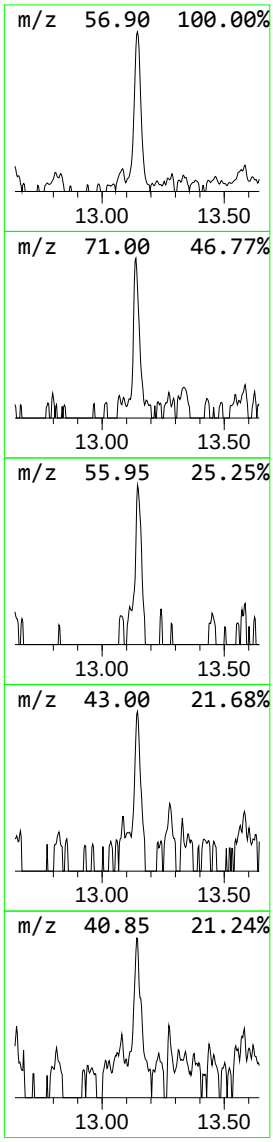
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.142	2.91 ug/L	15481	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	72
2	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	64
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
4	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	59
5	Nonane, 3-methyl-	142	C10H22	005911-04-6	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

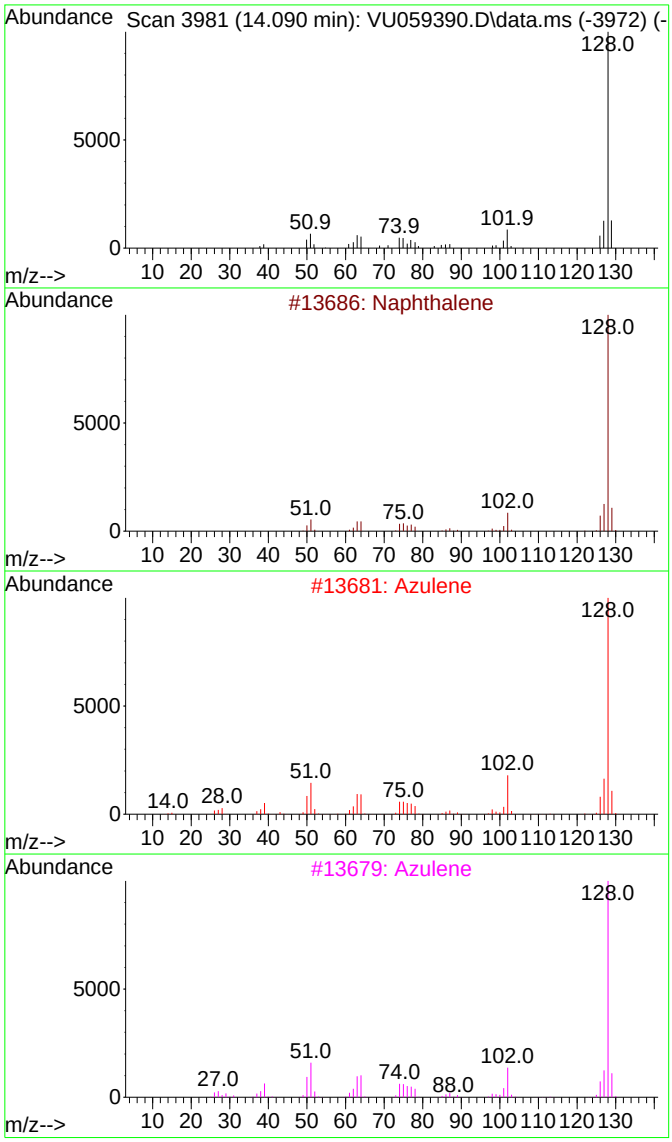
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

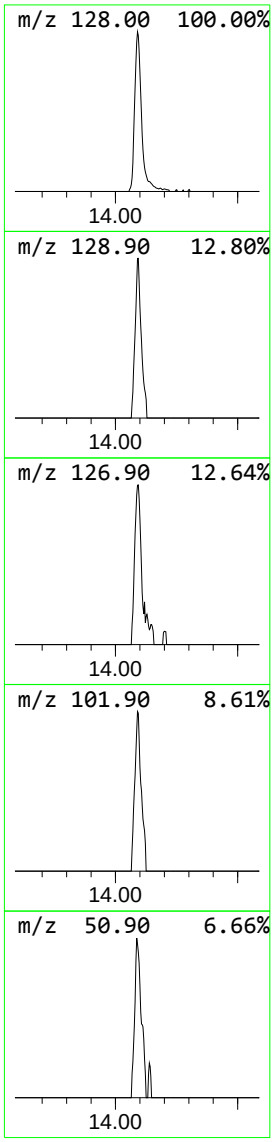
****

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.090	8.29 ug/L	44147	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	Azulene	128	C10H8	000275-51-4	91
3	Azulene	128	C10H8	000275-51-4	91
4	Naphthalene	128	C10H8	000091-20-3	91
5	Azulene	128	C10H8	000275-51-4	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

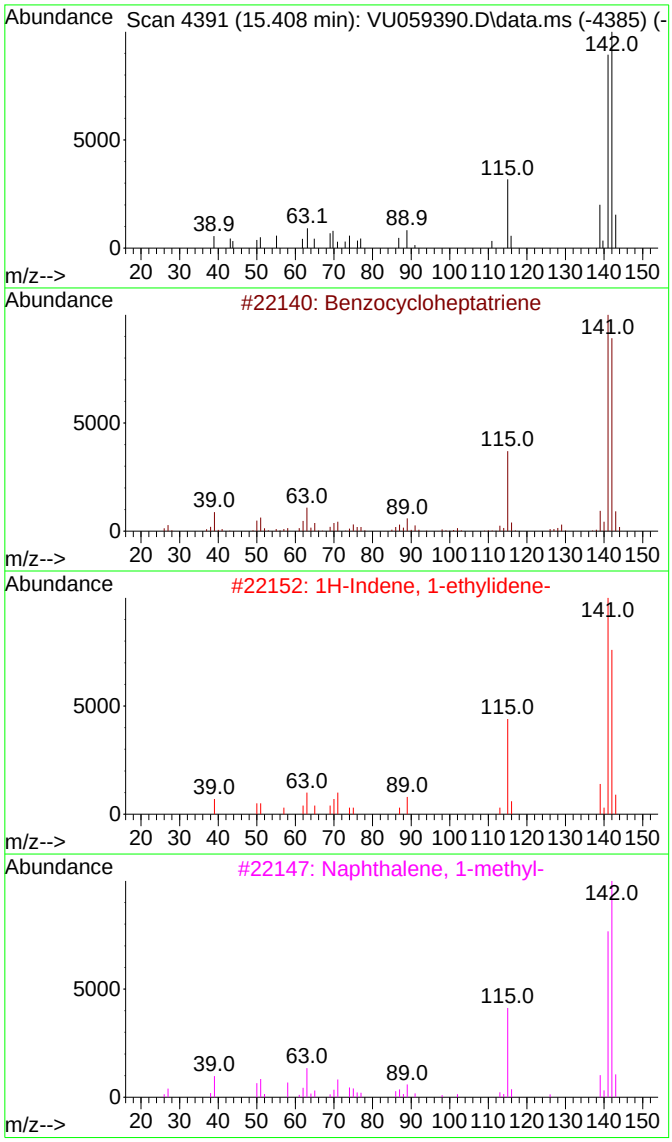
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

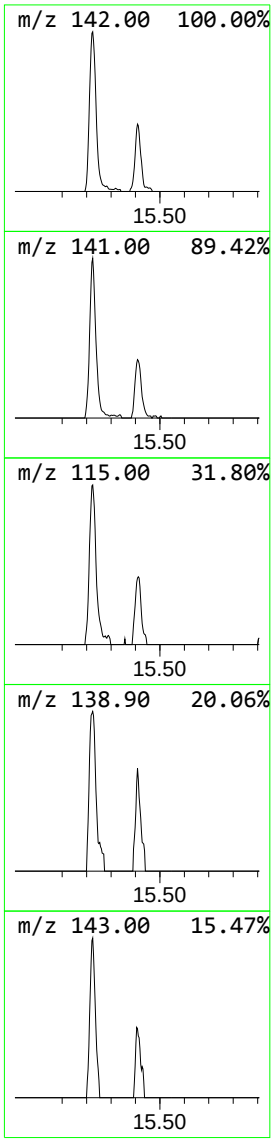
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzocycloheptatriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.408	3.86 ug/L	20539	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzocycloheptatriene	142	C11H10	000264-09-5	90
2	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87
3	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	87
4	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	86
5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	86





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

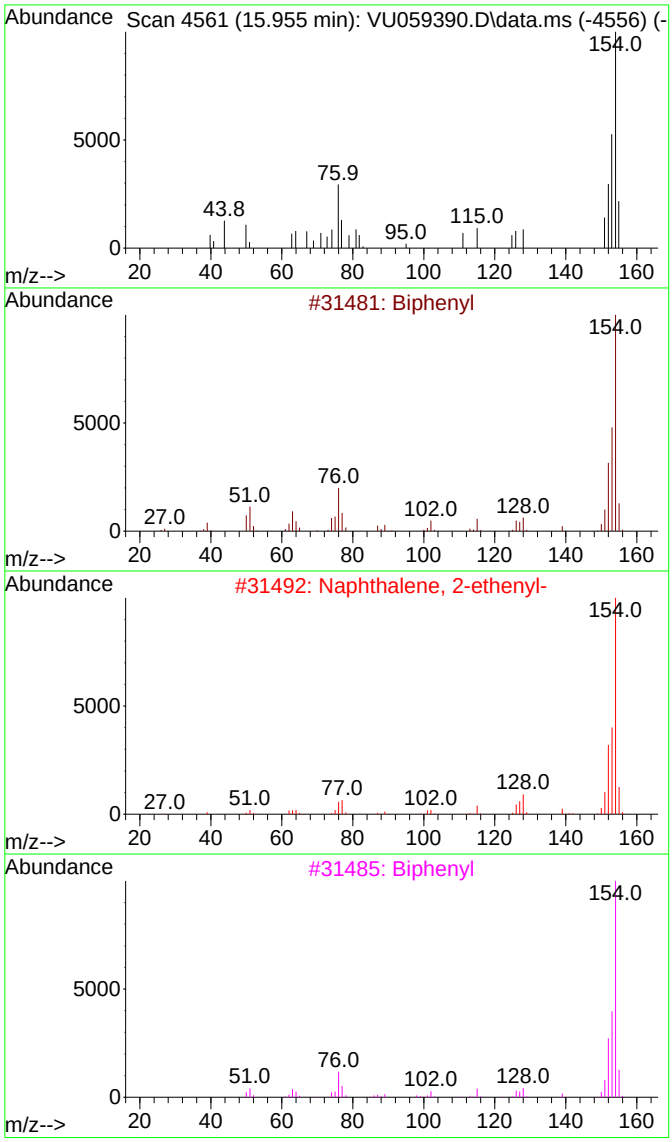
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

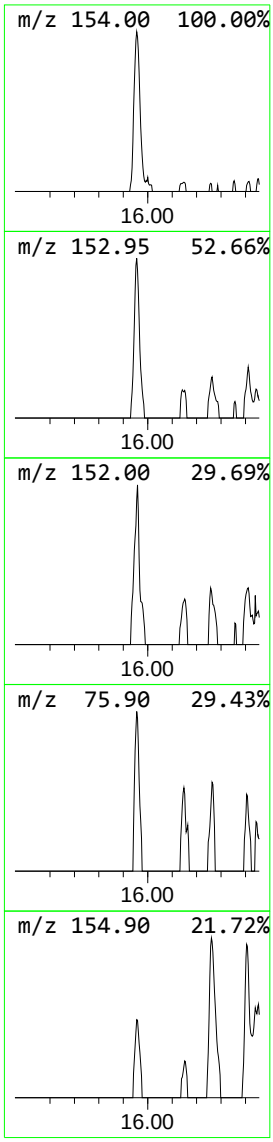
****

Peak Number 6 Naphthalene, 2-ethenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.955	2.74 ug/L	14562	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Biphenyl	154	C12H10	000092-52-4	72
2	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	64
3	Biphenyl	154	C12H10	000092-52-4	64
4	Biphenyl	154	C12H10	000092-52-4	59
5	Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

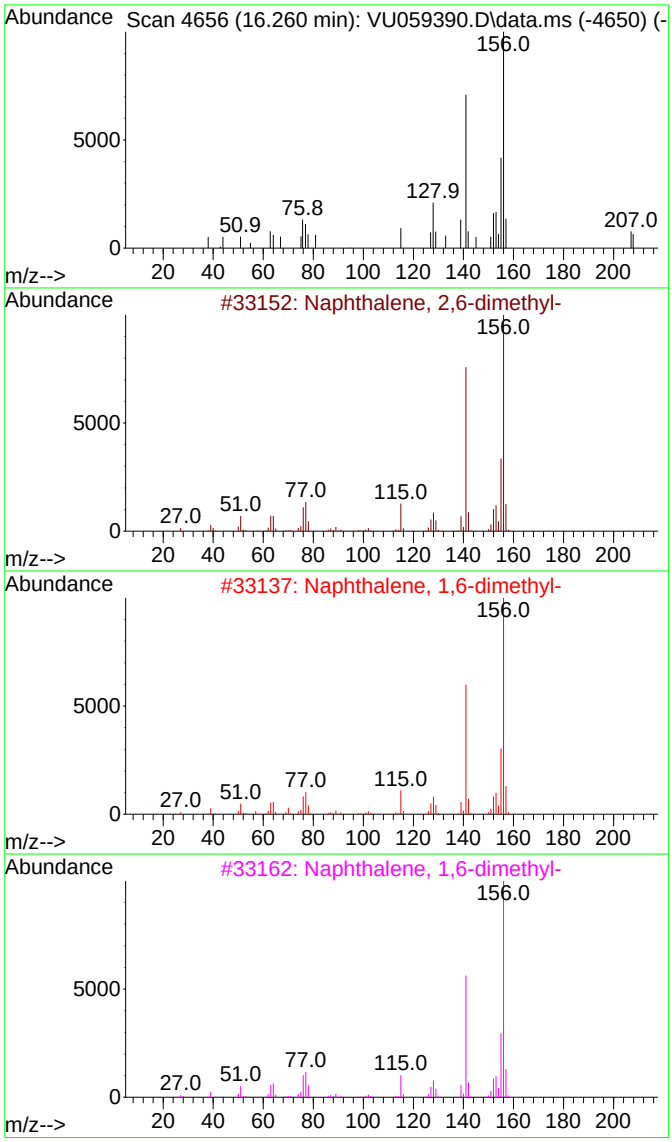
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

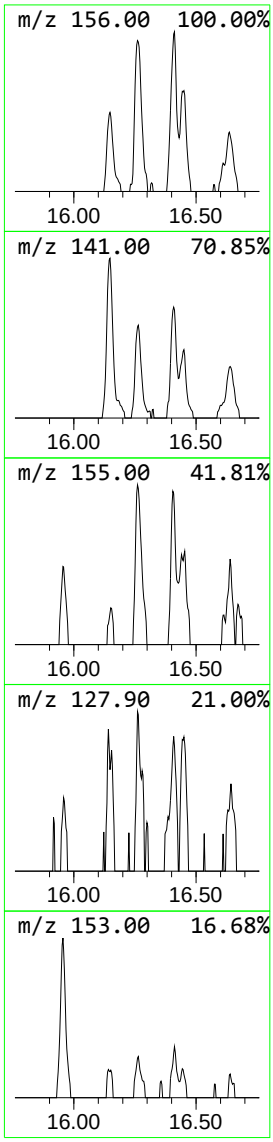
****

Peak Number 7 Naphthalene, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.260	2.67 ug/L	14207	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94
2	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
3	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
4	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

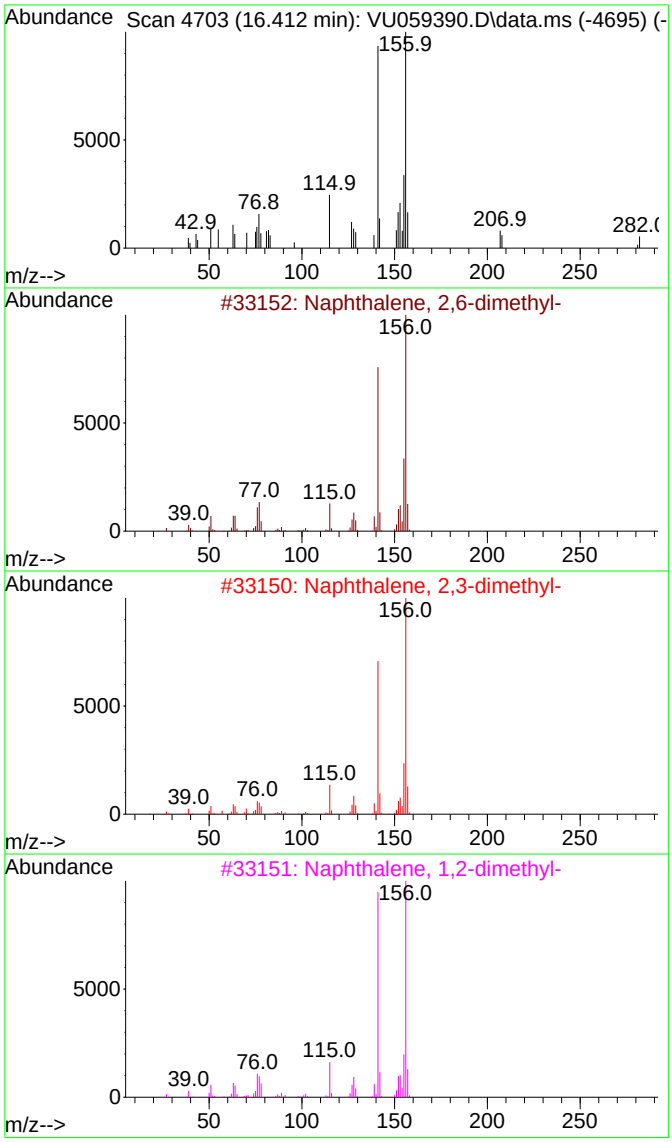
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

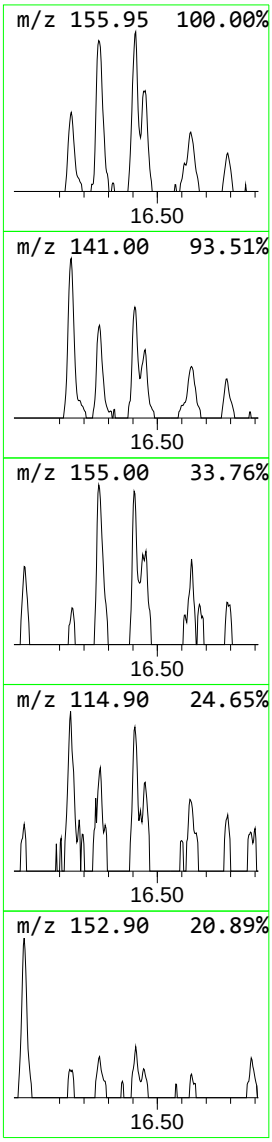
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.412	2.75 ug/L	14657	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	93
3	Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	93
4	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	92
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

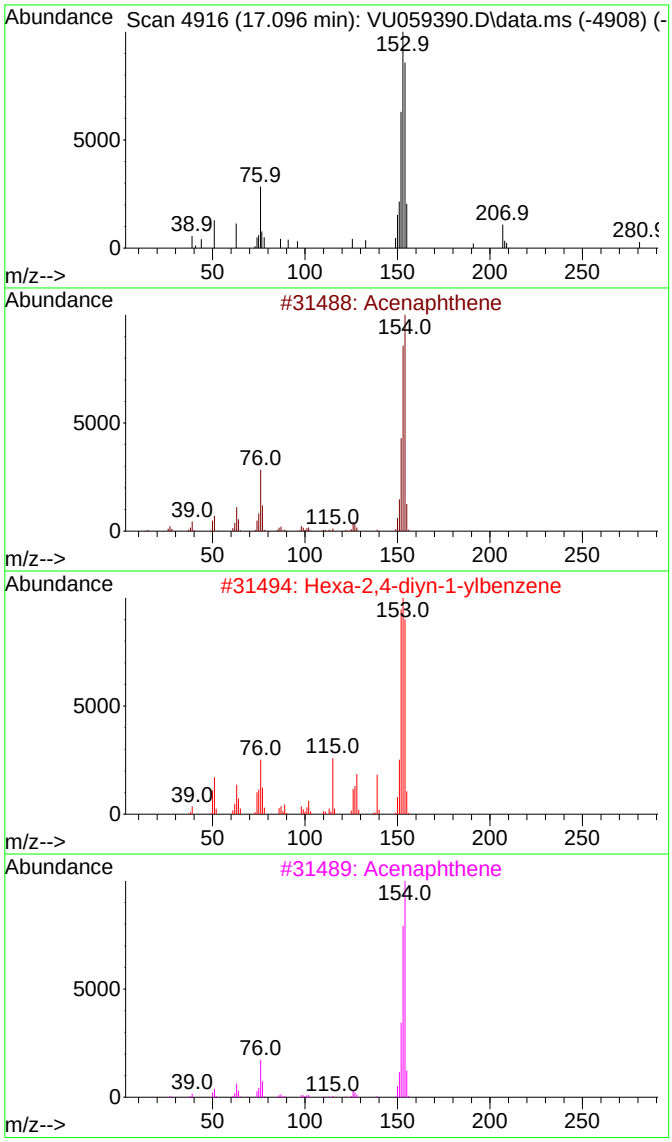
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

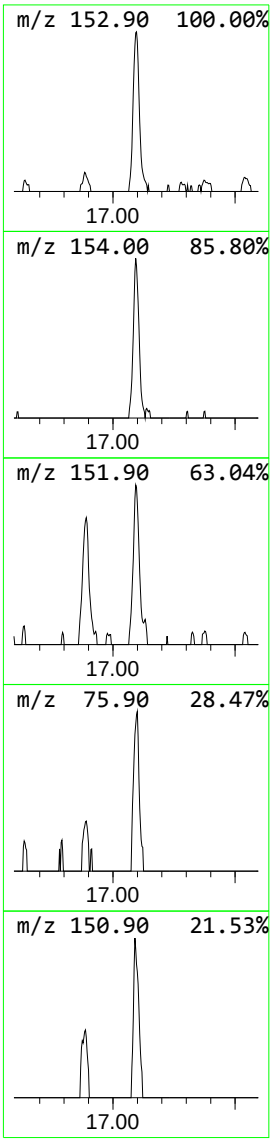
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.096	3.76 ug/L	20037	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acenaphthene	154	C12H10	000083-32-9	53
2	Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	53
3	Acenaphthene	154	C12H10	000083-32-9	50
4	1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	50
5	Acenaphthene	154	C12H10	000083-32-9	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059390.D
Acq On : 20 Jun 2024 19:27
Operator : MD/SY
Sample : P2909-02ME
Misc : 4.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B76ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	13.142	2.9	ug/L	15481	3	11.810	266207	50.0
Azulene	14.090	8.3	ug/L	44147	3	11.810	266207	50.0
Benzocyclohepta...	15.408	3.9	ug/L	20539	3	11.810	266207	50.0
Naphthalene, 2-...	15.955	2.7	ug/L	14562	3	11.810	266207	50.0
Naphthalene, 2,...	16.260	2.7	ug/L	14207	3	11.810	266207	50.0
Naphthalene, 2,...	16.412	2.8	ug/L	14657	3	11.810	266207	50.0
Hexa-2,4-diyn-1...	17.096	3.8	ug/L	20037	3	11.810	266207	50.0