

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059265.D
 Acq On : 14 Jun 2024 21:58
 Operator : MD/SY
 Sample : P2856-05ME
 Misc : 3.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SE9ME

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: VU059265.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	86	94	110	rBV	26582	43409	6.29%	0.629%
2	1.817	135	164	166	rBV3	46996	156549	22.68%	2.267%
3	2.476	366	369	376	rVB5	530	571	0.08%	0.008%
4	2.541	378	389	403	rVV	73295	119088	17.25%	1.724%
5	2.663	425	427	432	rVB3	843	668	0.10%	0.010%
6	2.820	471	476	478	rVB3	364	307	0.04%	0.004%
7	2.933	508	511	512	rBV2	452	257	0.04%	0.004%
8	3.026	530	540	552	rBV2	7978	15997	2.32%	0.232%
9	3.171	568	585	605	rBV	7225	20001	2.90%	0.290%
10	3.599	713	718	722	rVB2	249	266	0.04%	0.004%
11	3.679	736	743	747	rVV4	580	762	0.11%	0.011%
12	3.708	747	752	757	rVB2	248	300	0.04%	0.004%
13	3.965	829	832	838	rVB2	276	325	0.05%	0.005%
14	3.997	838	842	845	rBV2	290	305	0.04%	0.004%
15	4.097	868	873	876	rBV	231	249	0.04%	0.004%
16	4.274	923	928	937	rBV2	290	547	0.08%	0.008%
17	4.618	1025	1035	1083	rBV	81352	257745	37.34%	3.732%
18	4.881	1112	1117	1124	rBV4	355	428	0.06%	0.006%
19	5.052	1154	1170	1190	rBV	107271	245213	35.52%	3.551%
20	5.193	1208	1214	1217	rBV2	371	346	0.05%	0.005%
21	5.386	1271	1274	1280	rVV	309	349	0.05%	0.005%
22	5.711	1357	1375	1402	rBV3	192046	529559	76.71%	7.668%
23	5.968	1448	1455	1462	rBV6	1769	3153	0.46%	0.046%
24	6.238	1526	1539	1566	rBV	271975	530693	76.88%	7.685%
25	6.521	1619	1627	1640	rVB7	5422	10463	1.52%	0.152%
26	6.595	1640	1650	1664	rBV4	2370	5545	0.80%	0.080%
27	6.682	1664	1677	1703	rVB	139358	278270	40.31%	4.029%
28	7.132	1810	1817	1822	rBV2	206	258	0.04%	0.004%
29	7.196	1829	1837	1838	rBV2	1390	1177	0.17%	0.017%
30	7.232	1845	1848	1852	rVB3	855	614	0.09%	0.009%
31	7.264	1854	1858	1862	rBV2	272	313	0.05%	0.005%
32	7.560	1938	1950	1974	rBV	60330	112491	16.30%	1.629%
33	7.711	1993	1997	2002	rVB4	693	745	0.11%	0.011%
34	7.891	2039	2053	2071	rBV	193645	342974	49.68%	4.966%
35	8.177	2131	2142	2164	rBV	40692	76668	11.11%	1.110%
36	8.457	2226	2229	2234	rBV2	363	382	0.06%	0.006%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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

37	8.547	2245	2257	2273	rBV2	101002	172087	24.93%	2.492%
38	8.640	2273	2286	2326	rBV2	201707	503499	72.94%	7.291%
39	8.933	2375	2377	2385	rVB2	346	361	0.05%	0.005%
40	9.309	2490	2494	2500	rVV2	184	251	0.04%	0.004%
41	9.412	2513	2526	2558	rVV	382418	690323	100.00%	9.996%
42	9.566	2565	2574	2589	rVB	20221	35418	5.13%	0.513%
43	9.692	2603	2613	2638	rVB2	19774	37439	5.42%	0.542%
44	10.039	2717	2721	2725	rBV2	272	247	0.04%	0.004%
45	10.100	2730	2740	2750	rBV3	9450	15891	2.30%	0.230%
46	10.254	2782	2788	2793	rBV4	535	706	0.10%	0.010%
47	10.357	2813	2820	2822	rVB4	457	482	0.07%	0.007%
48	10.396	2827	2832	2835	rBV3	346	284	0.04%	0.004%
49	10.483	2854	2859	2864	rBV3	739	1014	0.15%	0.015%
50	10.614	2896	2900	2905	rBV3	545	500	0.07%	0.007%
51	10.753	2931	2943	2963	rBV	296222	499641	72.38%	7.235%
52	10.904	2981	2990	2993	rBV2	894	1356	0.20%	0.020%
53	10.939	2999	3001	3007	rVB2	613	437	0.06%	0.006%
54	11.000	3011	3020	3022	rBV3	4531	5682	0.82%	0.082%
55	11.090	3041	3048	3062	rVB4	5311	8747	1.27%	0.127%
56	11.190	3076	3079	3084	rBV2	284	310	0.04%	0.004%
57	11.219	3084	3088	3091	rVV2	332	359	0.05%	0.005%
58	11.261	3095	3101	3106	rVV2	338	502	0.07%	0.007%
59	11.293	3106	3111	3113	rVV	1213	1268	0.18%	0.018%
60	11.319	3117	3119	3123	rVV3	579	396	0.06%	0.006%
61	11.412	3141	3148	3154	rBV6	1496	1823	0.26%	0.026%
62	11.470	3155	3166	3180	rVB2	19553	30699	4.45%	0.445%
63	11.540	3180	3188	3201	rBV4	6772	10683	1.55%	0.155%
64	11.711	3235	3241	3244	rBV4	469	521	0.08%	0.008%
65	11.743	3248	3251	3260	rVB3	566	629	0.09%	0.009%
66	11.810	3260	3272	3290	rBV	400837	664713	96.29%	9.625%
67	11.891	3293	3297	3310	rVB3	7111	10791	1.56%	0.156%
68	11.955	3310	3317	3323	rBV4	1868	2518	0.36%	0.036%
69	12.093	3352	3360	3368	rBV3	3584	4920	0.71%	0.071%
70	12.190	3377	3390	3408	rBV	292717	473118	68.54%	6.851%
71	12.315	3418	3429	3442	rBV2	17309	29125	4.22%	0.422%
72	12.499	3482	3486	3495	rVB3	650	937	0.14%	0.014%
73	12.576	3506	3510	3517	rVB2	1183	1202	0.17%	0.017%
74	12.756	3559	3566	3576	rBV6	2832	4936	0.72%	0.071%
75	12.820	3583	3586	3590	rVB2	455	302	0.04%	0.004%
76	12.878	3600	3604	3607	rBV	487	323	0.05%	0.005%

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Integrator: RTE

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

77	12.974	3627	3634	3640	rBV2	1340	1510	0.22%	0.022%
78	13.019	3644	3648	3660	rVB2	1812	2469	0.36%	0.036%
79	13.164	3688	3693	3699	rVB4	812	1096	0.16%	0.016%
80	13.289	3729	3732	3734	rBV2	560	429	0.06%	0.006%
81	13.453	3770	3783	3793	rVB8	2234	4865	0.70%	0.070%
82	13.518	3793	3803	3814	rBV5	2861	4559	0.66%	0.066%
83	13.634	3828	3839	3850	rVB6	6075	10996	1.59%	0.159%
84	13.720	3863	3866	3871	rBV3	812	695	0.10%	0.010%
85	13.775	3881	3883	3889	rVB	444	313	0.05%	0.005%
86	13.846	3901	3905	3911	rVB3	761	655	0.09%	0.009%
87	14.080	3966	3978	4003	rBV	381325	634031	91.85%	9.181%
88	14.209	4011	4018	4028	rVB6	3706	5776	0.84%	0.084%
89	14.264	4032	4035	4037	rBV2	440	366	0.05%	0.005%
90	14.447	4088	4092	4097	rVB3	1261	1072	0.16%	0.016%
91	14.572	4124	4131	4134	rVV5	1136	1730	0.25%	0.025%
92	14.672	4158	4162	4164	rBV	508	363	0.05%	0.005%
93	14.724	4174	4178	4180	rBV4	647	581	0.08%	0.008%
94	15.010	4264	4267	4273	rBV2	465	482	0.07%	0.007%
95	15.164	4309	4315	4322	rBV2	1045	1676	0.24%	0.024%
96	15.222	4322	4333	4358	rVV	80913	138401	20.05%	2.004%
97	15.408	4380	4391	4408	rBV	61496	104788	15.18%	1.517%
98	15.961	4556	4563	4572	rBV3	2326	3896	0.56%	0.056%
99	16.267	4653	4658	4667	rBV7	2773	3545	0.51%	0.051%
100	16.408	4695	4702	4709	rBV5	6486	10253	1.49%	0.148%

Sum of corrected areas: 6905974

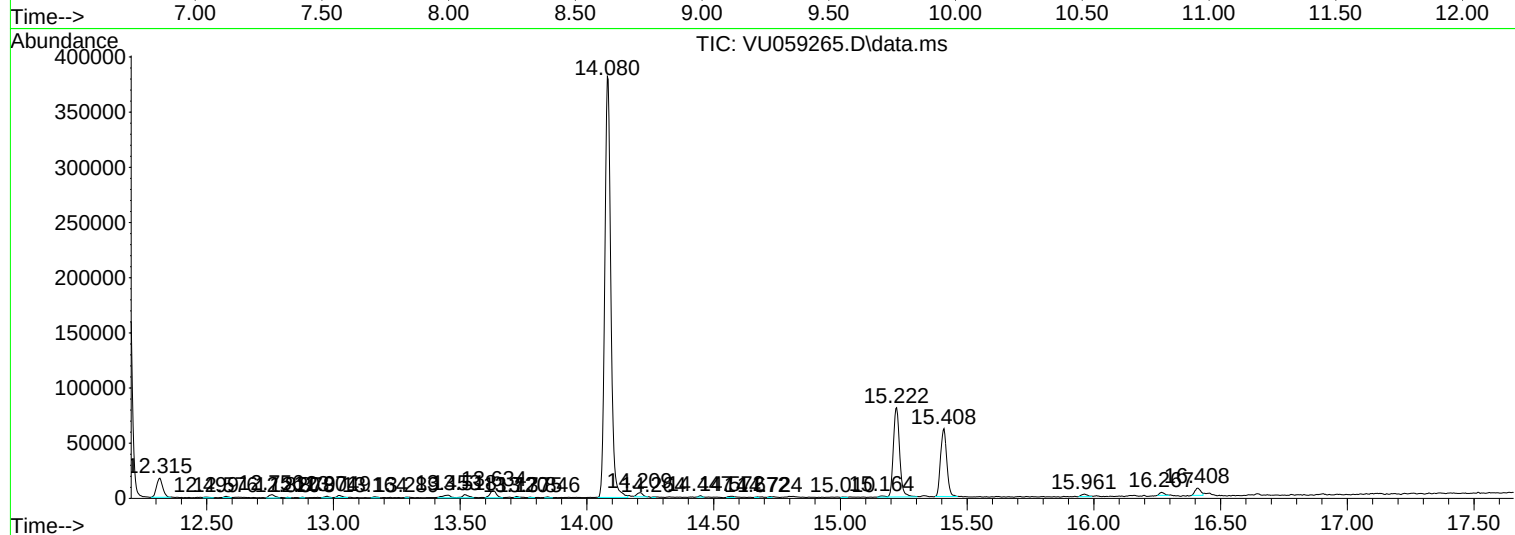
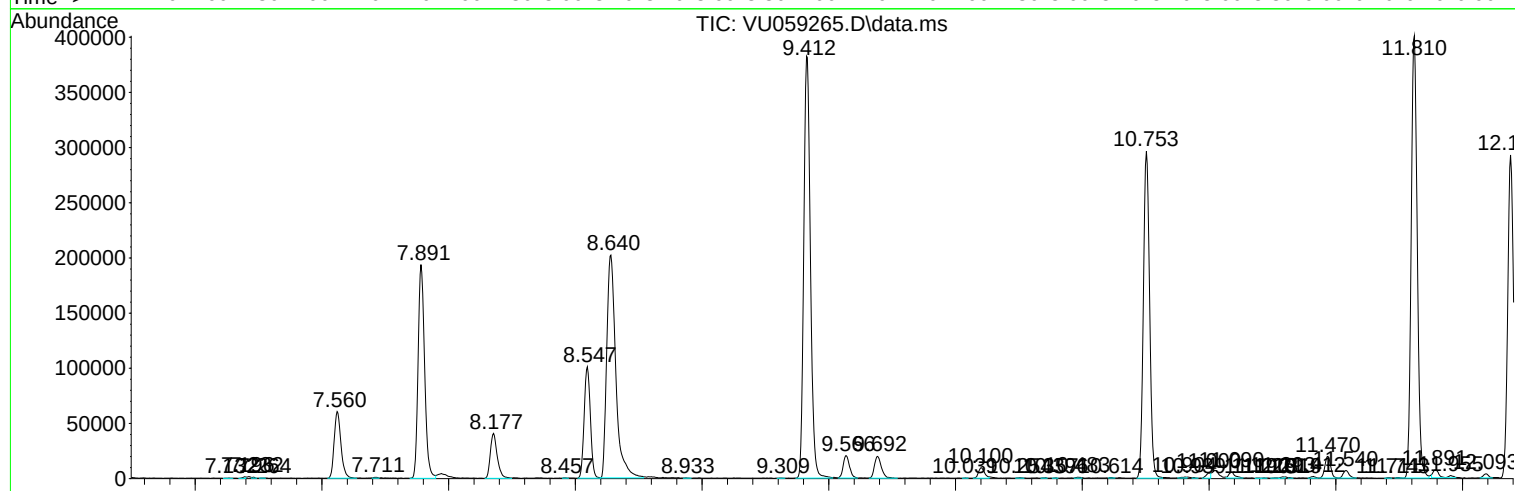
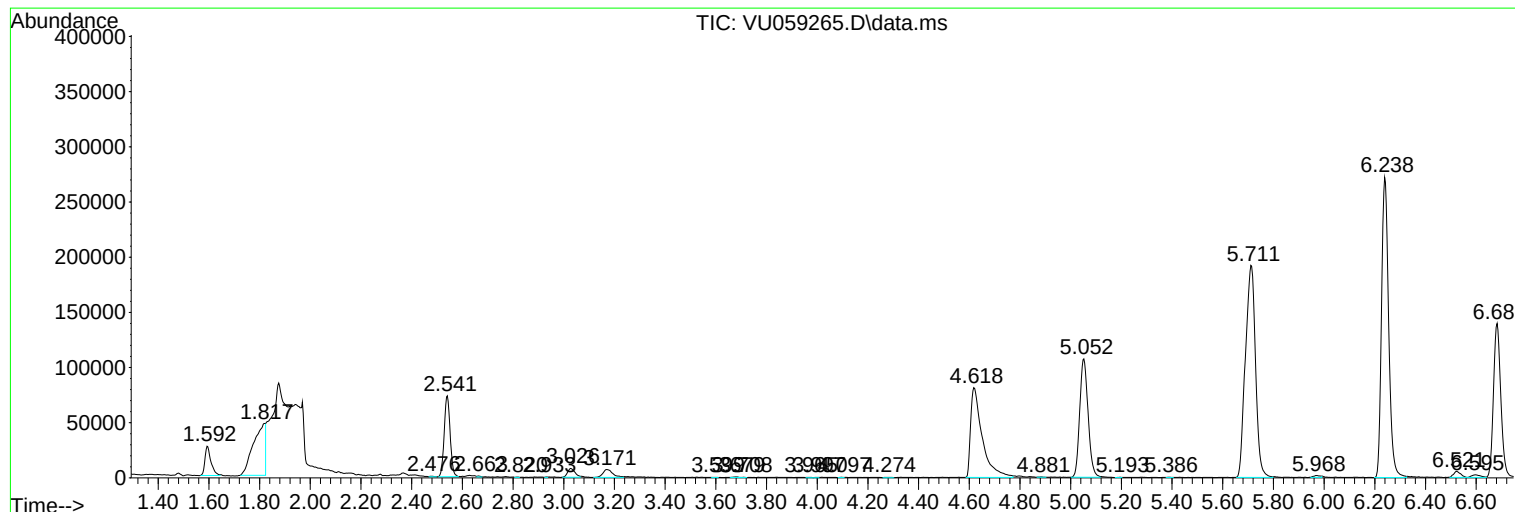
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_U
ClientSampleId :
C0SE9ME

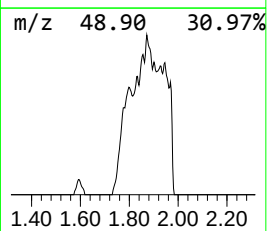
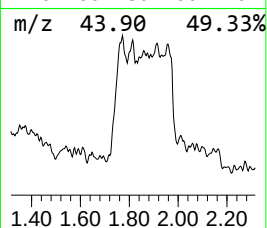
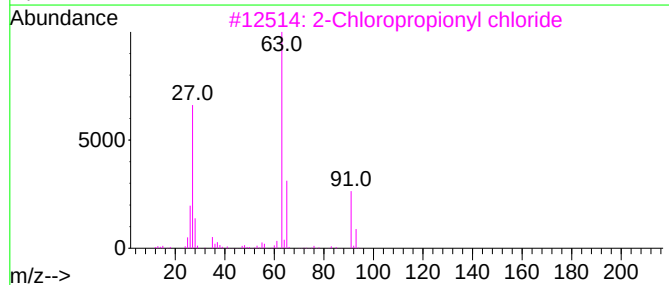
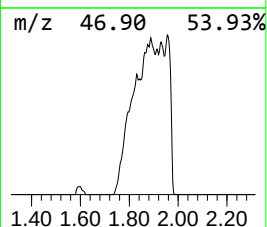
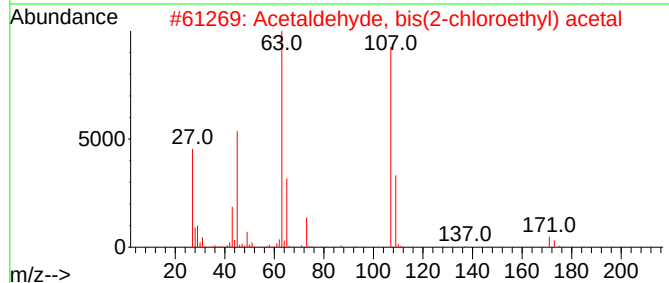
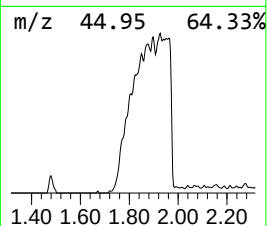
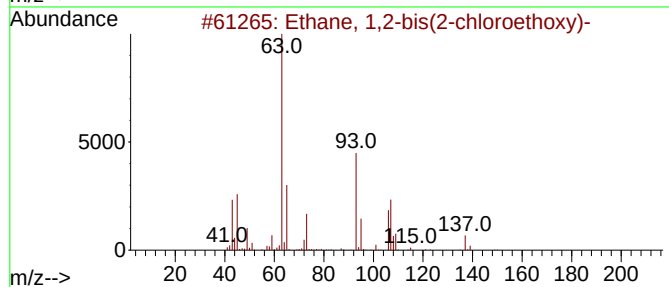
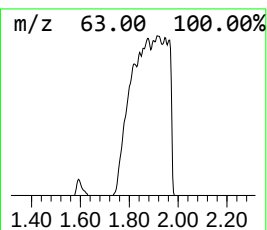
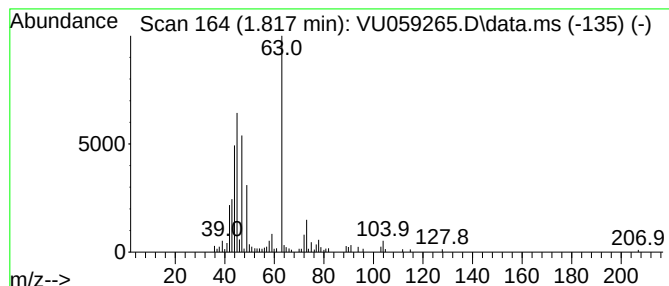
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.817	14.75 ug/L	156549	1,4-Difluorobenzene	6.238

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	39
2			Acetaldehyde, bis(2-chloroethyl)...	186	C6H12Cl2O2	014689-97-5	9
3			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	9
4			3,6,9,12-tetraoxatetradecane, 1,...	274	C10H20Cl2O4	1000401-80-9	9
5			N,N'-Bis(2-chloroethyl)oxamide	212	C6H10Cl2N2O2	016813-43-7	9



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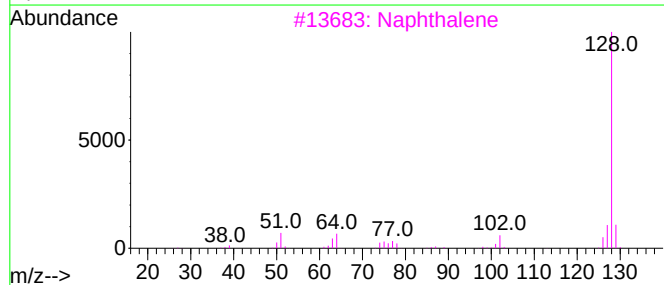
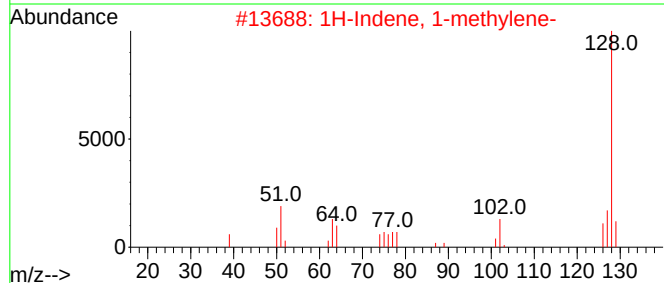
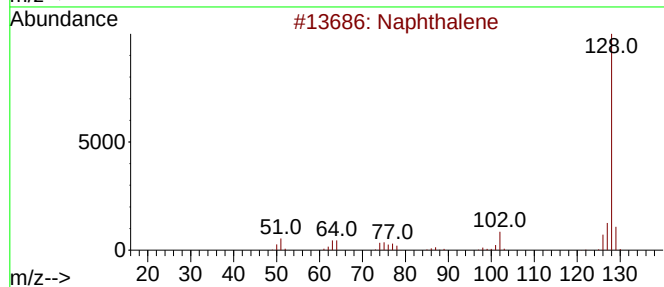
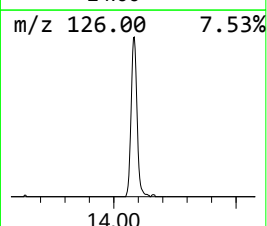
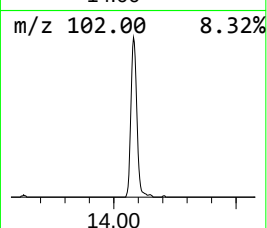
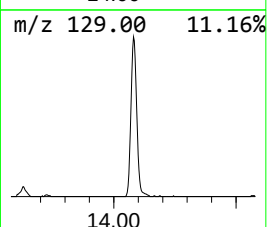
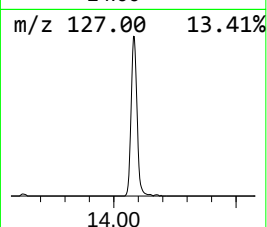
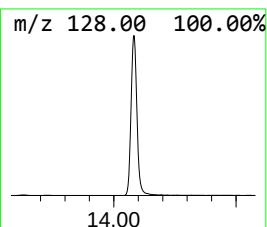
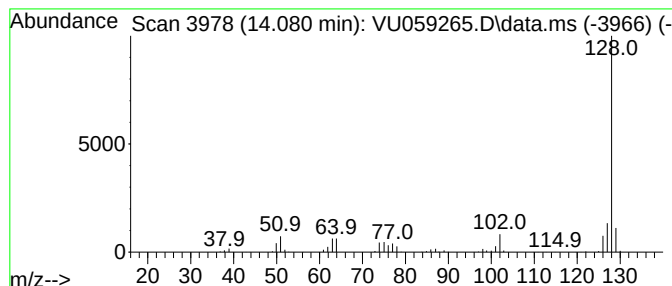
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Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.080	47.69 ug/L	634031	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Naphthalene	128	C10H8	000091-20-3	93
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.817	14.8	ug/L	156549	1	6.238	530693	50.0
Azulene	14.080	47.7	ug/L	634031	3	11.810	664713	50.0