

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY053123\
 Data File : VY013951.D
 Acq On : 31 May 2023 21:17
 Operator : KP/MD
 Sample : 02852-09RE
 Misc : 6.47g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CB-32-G3-SO-50.5-051823RE

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_Y\methods\82Y052323S.M
 Title : SW846 8260

Signal : TIC: VY013951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	6	7	15	rVB5	2146	3575	4.50%	0.729%
2	1.997	28	29	34	rVB2	801	879	1.11%	0.179%
3	2.125	47	50	53	rBV3	1076	1105	1.39%	0.225%
4	2.186	57	60	63	rBV2	772	1219	1.53%	0.249%
5	2.522	112	115	117	rVB4	1041	1345	1.69%	0.274%
6	2.546	117	119	124	rVB5	833	930	1.17%	0.190%
7	2.619	129	131	133	rBV3	1030	1015	1.28%	0.207%
8	2.662	135	138	139	rBV2	973	872	1.10%	0.178%
9	2.820	161	164	167	rBV4	708	1169	1.47%	0.239%
10	2.851	167	169	173	rVV4	794	1057	1.33%	0.216%
11	3.003	192	194	197	rBV2	719	909	1.14%	0.185%
12	3.174	217	222	227	rVB5	1000	1061	1.33%	0.216%
13	3.259	227	236	246	rBV5	2677	7274	9.15%	1.484%
14	3.954	345	350	351	rBV3	1279	1999	2.51%	0.408%
15	3.972	351	353	357	rVB3	827	920	1.16%	0.188%
16	4.722	467	476	486	rBV4	2804	8702	10.94%	1.775%
17	5.740	638	643	644	rBV3	855	1066	1.34%	0.217%
18	5.942	671	676	678	rBV2	418	832	1.05%	0.170%
19	6.966	836	844	845	rBV3	722	1329	1.67%	0.271%
20	7.508	927	933	938	rVB3	803	1726	2.17%	0.352%
21	7.722	959	968	974	rVV2	12939	31783	39.97%	6.485%
22	7.795	974	980	988	rVB2	25032	57448	72.24%	11.721%
23	8.149	1029	1038	1046	rBV3	12626	28243	35.52%	5.763%
24	8.557	1100	1105	1111	rVB6	2416	5228	6.57%	1.067%
25	8.697	1120	1128	1138	rBV	32766	63425	79.76%	12.941%
26	8.911	1158	1163	1164	rBV2	848	1106	1.39%	0.226%
27	8.947	1164	1169	1174	rVB4	1928	3504	4.41%	0.715%
28	9.673	1282	1288	1290	rBV2	433	812	1.02%	0.166%
29	10.185	1365	1372	1379	rBV	44741	79519	100.00%	16.224%
30	10.374	1396	1403	1409	rBV4	5557	10125	12.73%	2.066%
31	10.941	1490	1496	1503	rBV3	1818	3928	4.94%	0.801%
32	11.496	1580	1587	1594	rBV	38150	66040	83.05%	13.474%
33	11.898	1646	1653	1658	rBV6	1895	3947	4.96%	0.805%
34	12.483	1743	1749	1756	rBV	25332	40946	51.49%	8.354%
35	12.922	1816	1821	1825	rBV3	817	1676	2.11%	0.342%
36	13.343	1888	1890	1895	rVB3	931	863	1.09%	0.176%

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37	13.428	1898	1904	1912	rVB	27752	43504	54.71%	8.876%
38	13.526	1917	1920	1925	rBV5	730	1144	1.44%	0.233%
39	13.782	1958	1962	1964	rBV3	892	911	1.15%	0.186%
40	13.958	1985	1991	1996	rVB4	1346	2479	3.12%	0.506%
41	14.208	2028	2032	2037	rBV5	1216	2496	3.14%	0.509%
42	15.489	2241	2242	2247	rVB3	824	854	1.07%	0.174%
43	15.818	2293	2296	2299	rBV3	777	1152	1.45%	0.235%

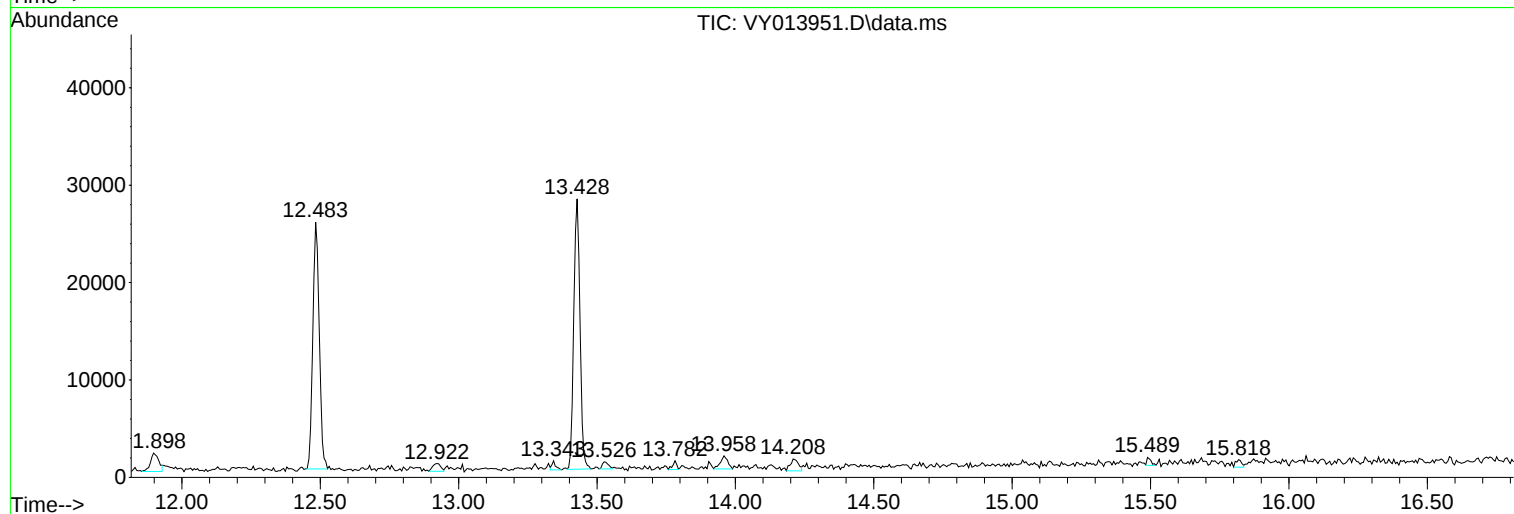
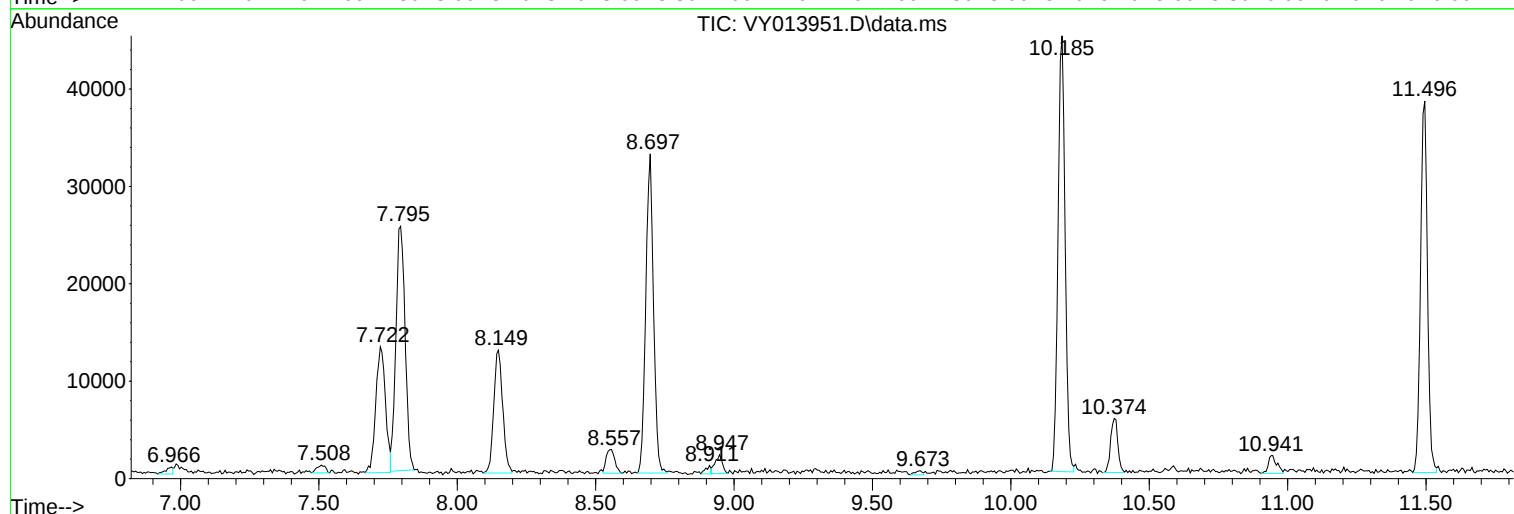
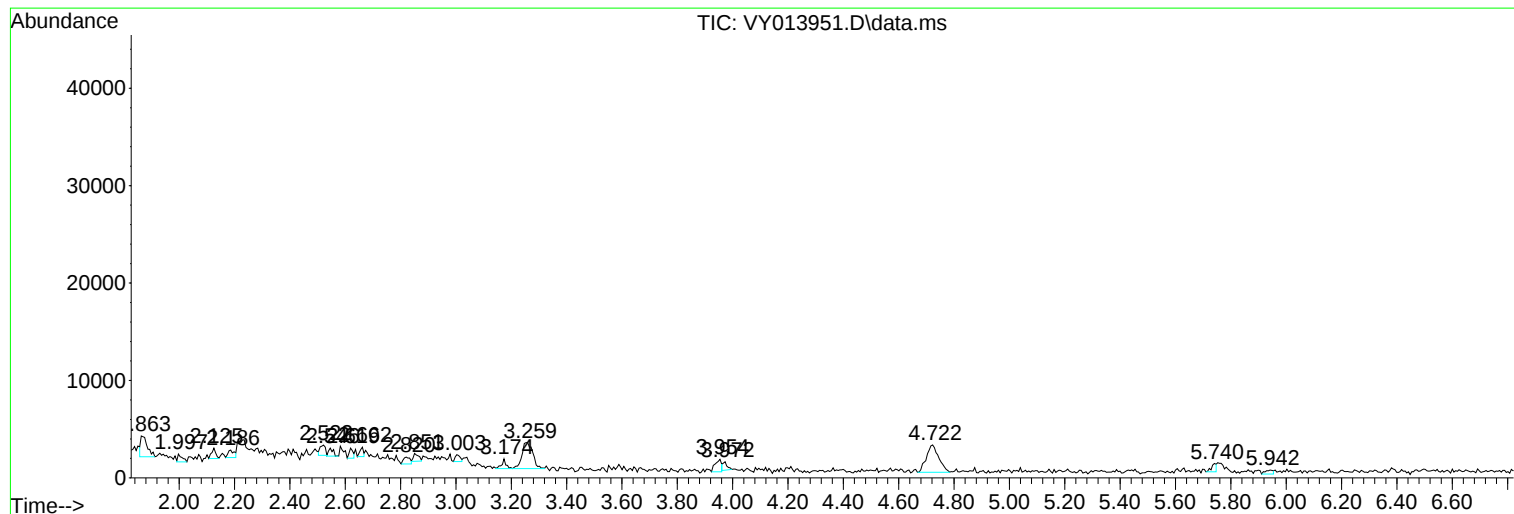
Sum of corrected areas: 490117

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052323S.M
Quant Title : SW846 8260

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



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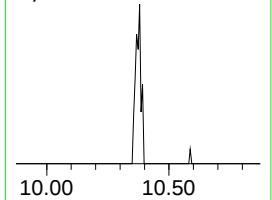
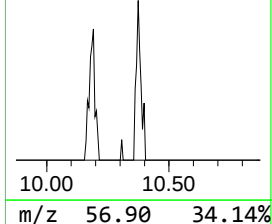
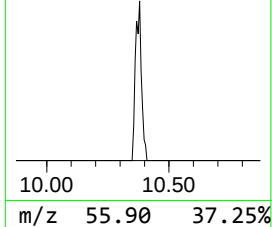
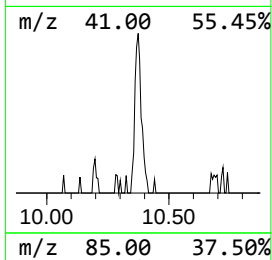
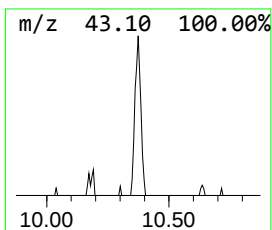
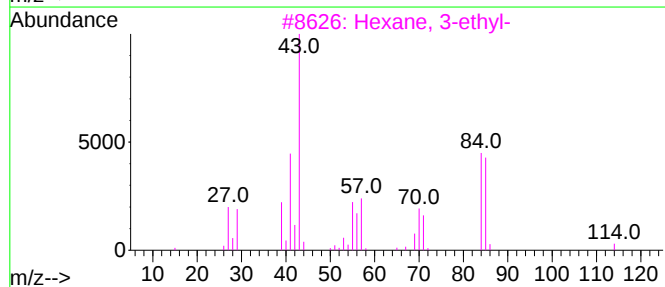
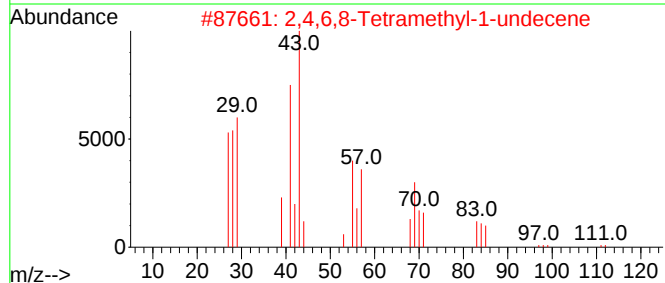
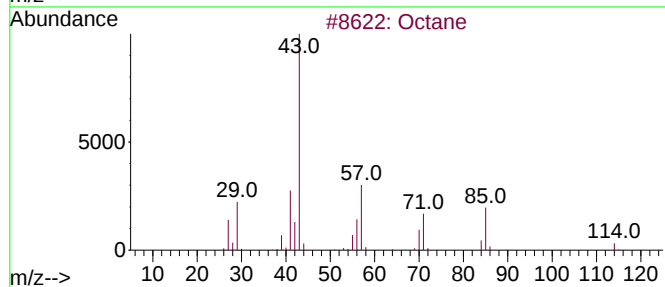
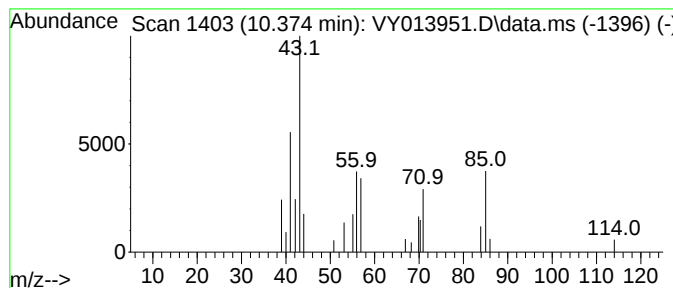
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052323S.M
Quant Title : SW846 8260

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

Peak Number 3 Octane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.374	7.67 ug/l	10125	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane	114	C8H18	000111-65-9	72
2			2,4,6,8-Tetramethyl-1-undecene	210	C15H30	059920-26-2	50
3			Hexane, 3-ethyl-	114	C8H18	000619-99-8	45
4			Pyrrolidine	71	C4H9N	000123-75-1	38
5			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octane	10.374	7.7	ug/l	10125	3	11.489	66040	50.0