

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN063020\
 Data File : VN062245.D
 Acq On : 30 Jun 2020 17:27
 Operator : JC/MD
 Sample : L3152-03
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DRUM-COMP

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.130	102	111	120	rBV3	10549	18860	1.64%	0.250%
2	2.420	182	201	202	rBV7	17768	38599	3.36%	0.512%
3	4.490	829	845	855	rBV6	4973	13643	1.19%	0.181%
4	7.545	1777	1795	1806	rBV3	137281	372416	32.37%	4.939%
5	7.619	1807	1818	1835	rVV	237763	595562	51.77%	7.899%
6	7.696	1836	1842	1856	rVB5	11025	24391	2.12%	0.323%
7	7.828	1864	1883	1899	rBV3	37667	92283	8.02%	1.224%
8	7.985	1914	1932	1954	rBV2	163427	387821	33.71%	5.144%
9	8.111	1959	1971	1983	rVB7	7650	17457	1.52%	0.232%
10	8.397	2046	2060	2075	rVB3	33616	70810	6.16%	0.939%
11	8.548	2090	2107	2130	rBV	396768	820342	71.31%	10.880%
12	9.043	2242	2261	2272	rBV6	9381	24321	2.11%	0.323%
13	10.059	2557	2577	2588	rBV	629552	1150417	100.00%	15.258%
14	10.123	2588	2597	2616	rVB	236565	434561	37.77%	5.763%
15	11.381	2974	2988	3013	rBV	564885	983772	85.51%	13.048%
16	12.377	3285	3298	3320	rVB	385704	656956	57.11%	8.713%
17	12.705	3389	3400	3410	rVB4	22316	35793	3.11%	0.475%
18	13.017	3486	3497	3506	rVB3	18011	28482	2.48%	0.378%
19	13.200	3542	3554	3563	rBV3	17029	35787	3.11%	0.475%
20	13.319	3579	3591	3609	rBV	480438	819408	71.23%	10.868%
21	13.561	3662	3666	3675	rVB3	11166	14946	1.30%	0.198%
22	13.647	3684	3693	3702	rBV3	32117	49086	4.27%	0.651%
23	13.863	3754	3760	3769	rVB2	17859	27176	2.36%	0.360%
24	13.969	3784	3793	3802	rBV6	12383	20759	1.80%	0.275%
25	14.146	3840	3848	3855	rBV6	12149	24159	2.10%	0.320%
26	14.223	3867	3872	3880	rVB	17584	25778	2.24%	0.342%
27	14.278	3880	3889	3892	rBV6	18493	28731	2.50%	0.381%
28	14.361	3907	3915	3921	rVB10	7806	12343	1.07%	0.164%
29	14.454	3937	3944	3950	rBV3	10991	19810	1.72%	0.263%
30	14.499	3952	3958	3967	rVV3	33845	48931	4.25%	0.649%
31	14.564	3968	3978	3988	rVV6	36442	81020	7.04%	1.075%
32	14.618	3989	3995	4007	rVB4	19187	33208	2.89%	0.440%
33	14.725	4021	4028	4033	rBV8	6919	11770	1.02%	0.156%
34	14.827	4053	4060	4065	rBV4	19435	26240	2.28%	0.348%

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Integration Parameters: RTEINT.P

Integrator: RTE
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Start Thrs: 0.2 Max Peaks: 100
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35	14.930	4084	4092	4104	rVB9	18667	37039	3.22%	0.491%
36	15.110	4136	4148	4149	rBV2	11530	20938	1.82%	0.278%
37	15.210	4170	4179	4190	rBV2	24696	52757	4.59%	0.700%
38	15.387	4225	4234	4247	rBV5	18991	38504	3.35%	0.511%
39	15.741	4334	4344	4364	rVB6	15309	43259	3.76%	0.574%
40	15.860	4367	4381	4397	rBV2	69487	158036	13.74%	2.096%
41	16.062	4438	4444	4453	rVB8	11872	20124	1.75%	0.267%
42	16.123	4454	4463	4486	rVB	33775	70347	6.11%	0.933%
43	16.313	4511	4522	4536	rBV4	21678	53259	4.63%	0.706%

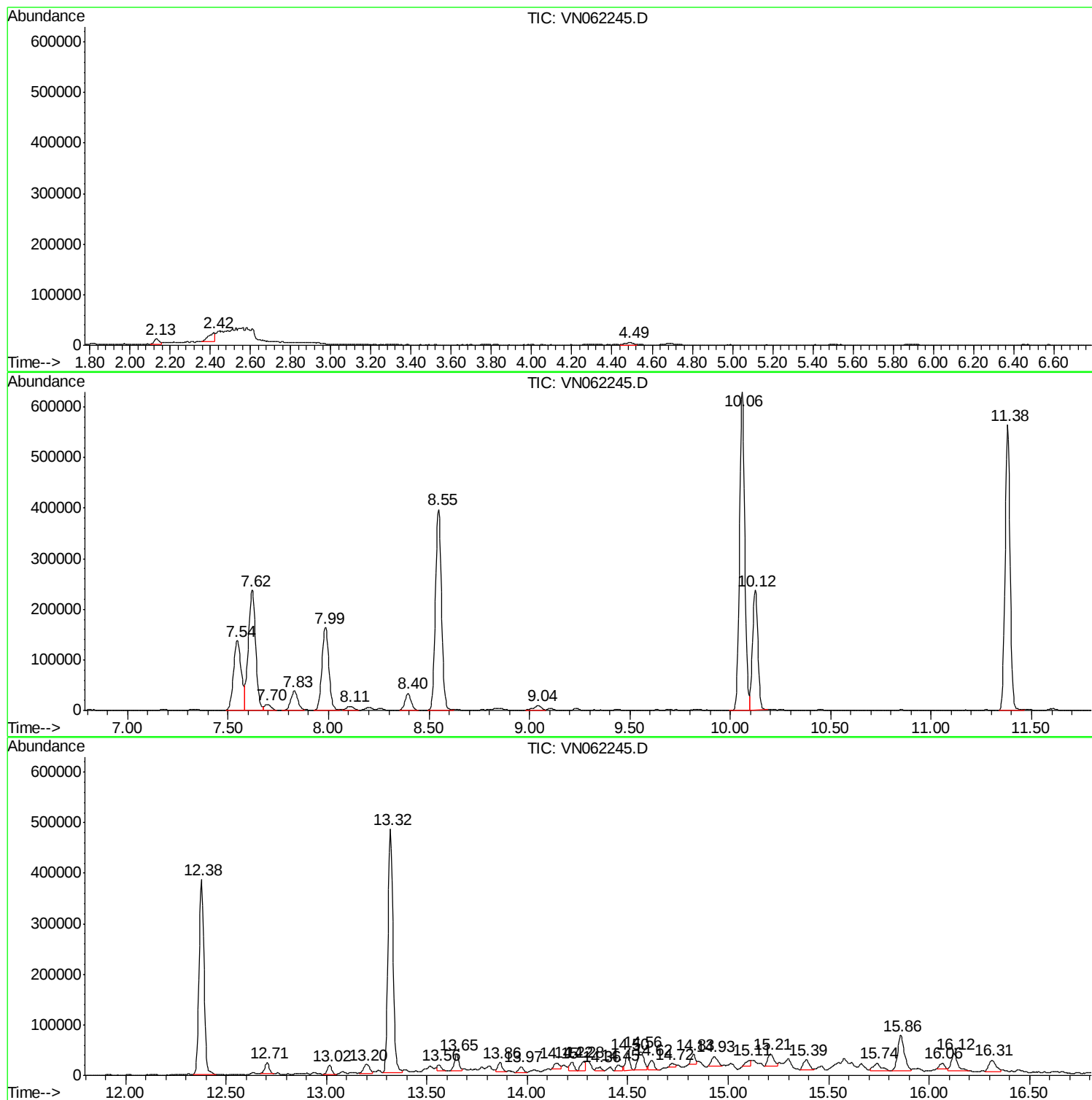
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_N\METHODS\82N062420W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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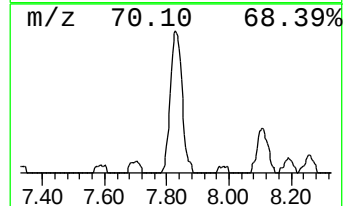
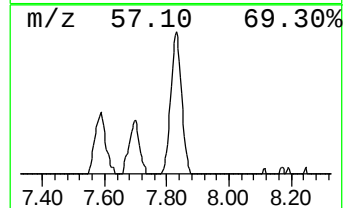
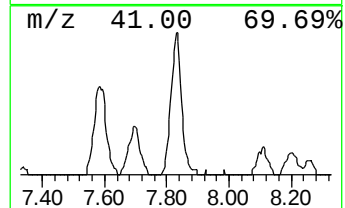
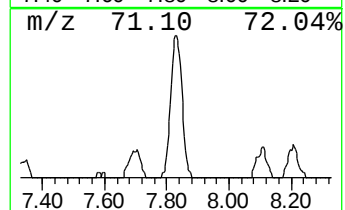
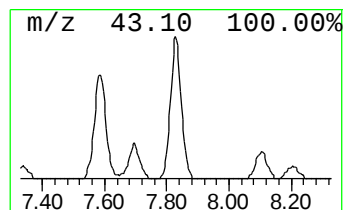
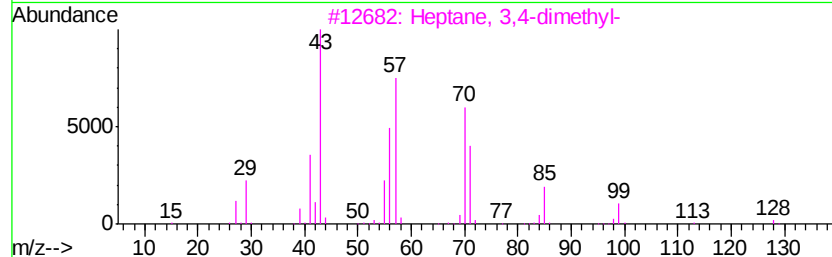
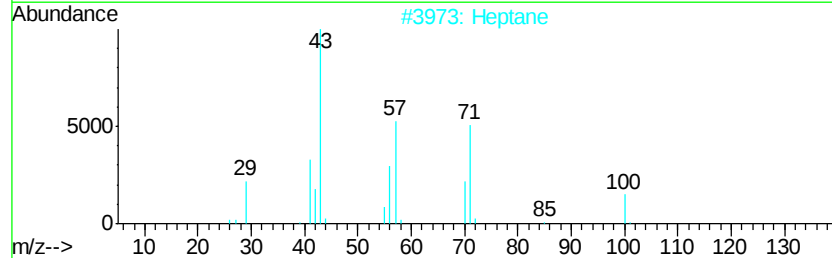
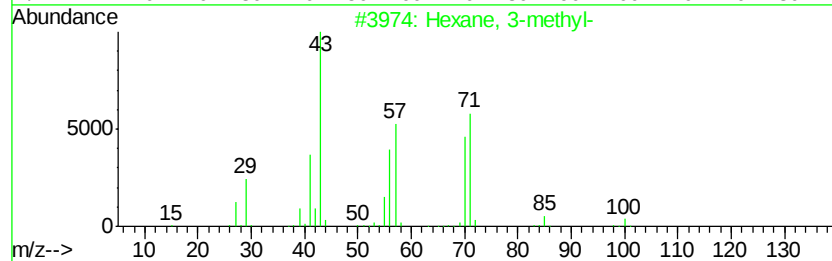
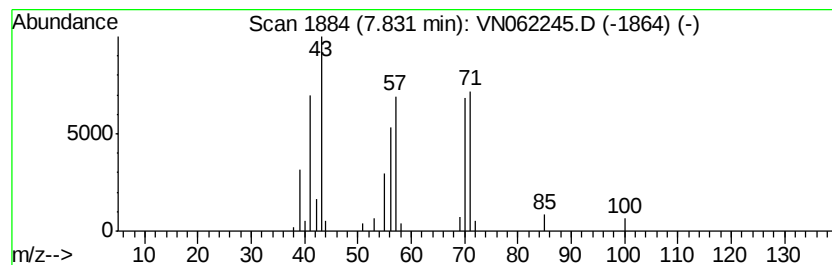
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.83	7.75 ug/l	92283	Pentafluorobenzene	7.62		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-		100	C7H16	000589-34-4	91
2	Heptane		100	C7H16	000142-82-5	72
3	Heptane, 3,4-dimethyl-		128	C9H20	000922-28-1	64
4	Decane, 3,3,4-trimethyl-		184	C13H28	049622-18-6	59
5	Octane, 4,5-dimethyl-		142	C10H22	015869-96-2	59



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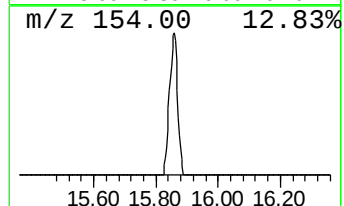
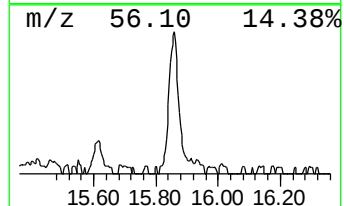
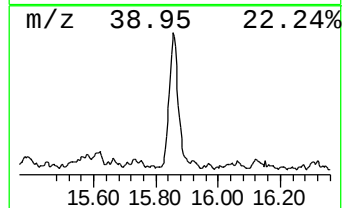
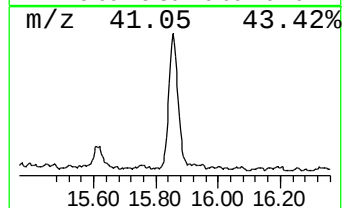
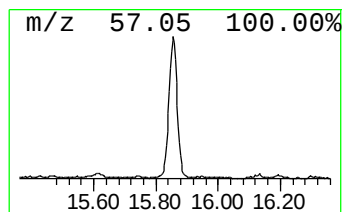
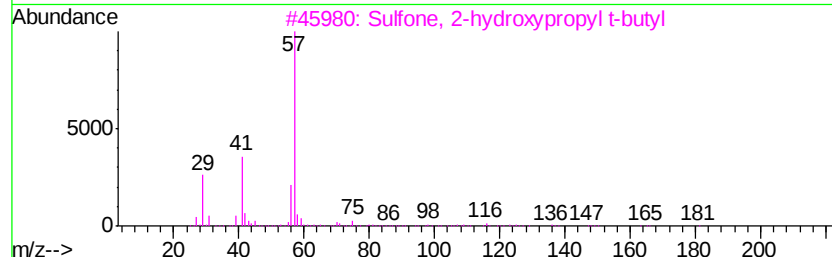
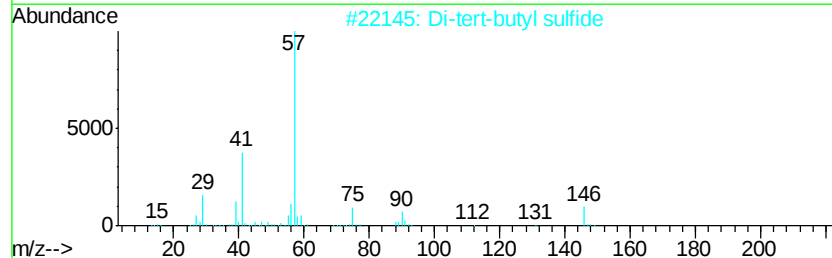
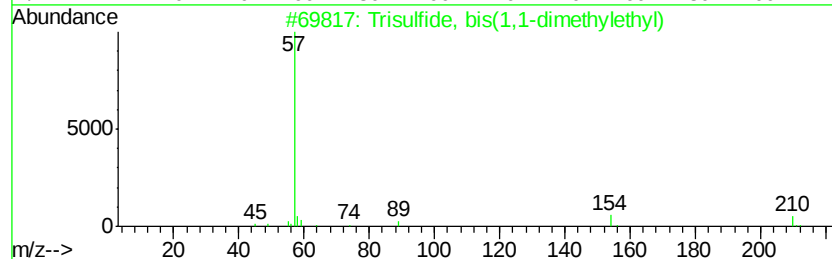
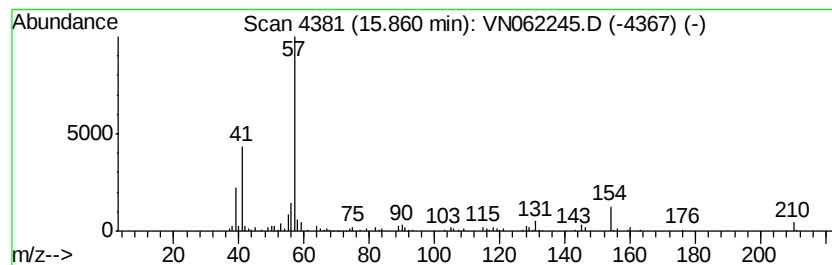
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Peak Number 2 Trisulfide, bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.86	9.64 ug/l	158036	1,4-Dichlorobenzene-d4	13.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	52
2	Di-tert-butyl sulfide	146	C8H18S	000107-47-1	47
3	Sulfone, 2-hydroxypropyl t-butyl	180	C7H16O3S	154619-05-3	32
4	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AqO2	007324-58-5	32
5	Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexane, 3-methyl-	7.83	7.8	ug/l	92283	1	7.62	595562	50.0
Trisulfide, bis(1...	15.86	9.6	ug/l	158036	4	13.32	819408	50.0