

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051822\
 Data File : VY008838.D
 Acq On : 19 May 2022 01:25
 Operator : KP/MD
 Sample : N2869-11
 Misc : 5.76g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 P031-SS001-0006-01

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\82Y051722S.M
 Title : SW846 8260

Signal : TIC: VY008838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.027	354	362	373	rBV3	4715	13180	1.66%	0.279%
2	4.716	466	475	492	rVB2	7082	20738	2.61%	0.439%
3	5.746	636	644	651	rBV5	2828	8202	1.03%	0.174%
4	6.984	838	847	861	rBV	8278	32675	4.11%	0.692%
5	7.716	956	967	973	rBV	107628	256626	32.26%	5.431%
6	7.789	973	979	991	rVB	168297	372708	46.86%	7.888%
7	8.136	1024	1036	1049	rVB2	111825	286517	36.02%	6.064%
8	8.691	1118	1127	1136	rBV	271632	525112	66.02%	11.113%
9	10.179	1363	1371	1379	rBV	466395	755125	94.93%	15.981%
10	10.581	1430	1437	1444	rBV	38016	66386	8.35%	1.405%
11	10.947	1486	1497	1509	rBV	23808	48178	6.06%	1.020%
12	11.313	1551	1557	1563	rBV2	5487	9796	1.23%	0.207%
13	11.489	1577	1586	1597	rBV	428297	670739	84.32%	14.195%
14	12.483	1739	1749	1758	rBV3	443078	795423	100.00%	16.834%
15	12.623	1769	1772	1778	rBV3	5450	10088	1.27%	0.213%
16	12.831	1798	1806	1812	rBV8	7622	17844	2.24%	0.378%
17	13.068	1830	1845	1852	rVB	19039	40558	5.10%	0.858%
18	13.178	1857	1863	1872	rBV2	10246	16840	2.12%	0.356%
19	13.282	1872	1880	1889	rBV	39114	70310	8.84%	1.488%
20	13.428	1895	1904	1909	rBV	397760	616515	77.51%	13.048%
21	13.477	1909	1912	1923	rVB2	28859	61068	7.68%	1.292%
22	13.641	1930	1939	1946	rBV2	9326	19009	2.39%	0.402%
23	13.965	1985	1992	1998	rVB3	6510	11498	1.45%	0.243%

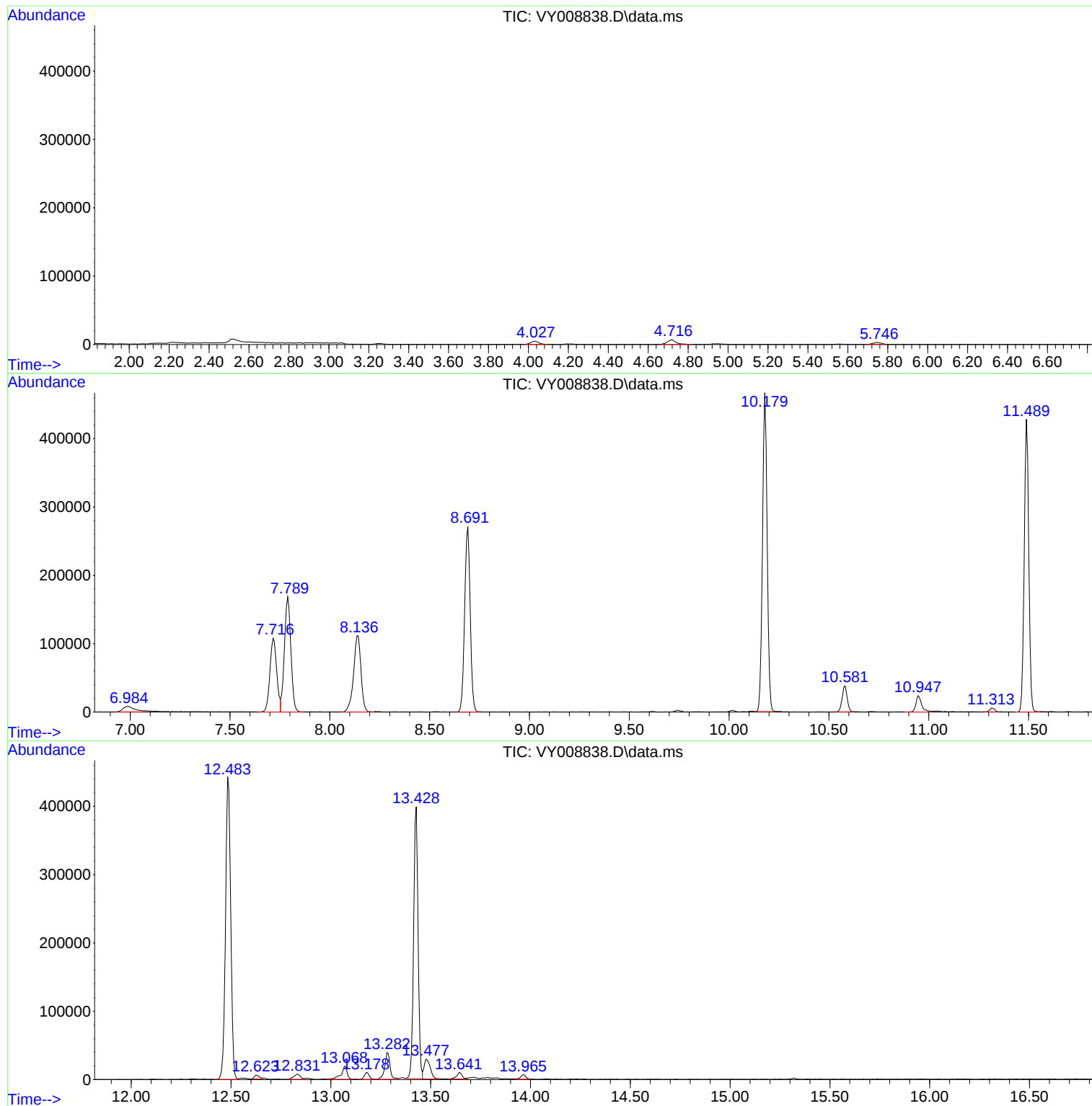
Sum of corrected areas: 4725135

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051722S.M
Quant Title : SW846 8260

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



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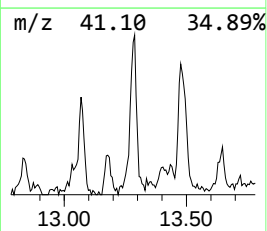
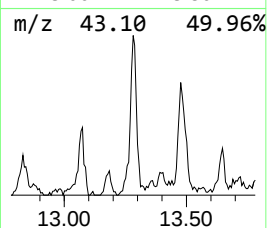
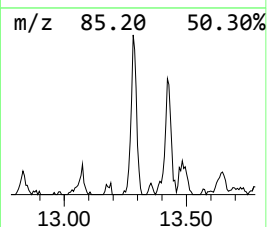
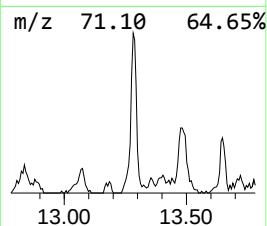
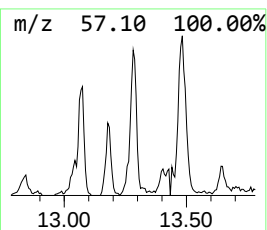
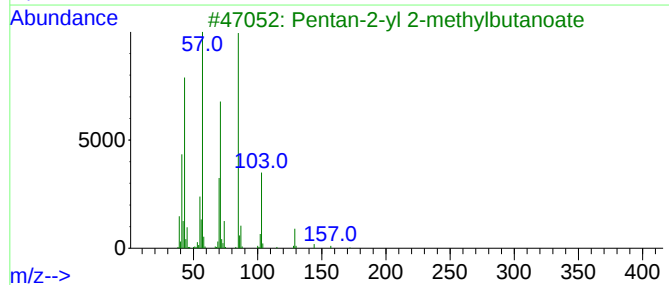
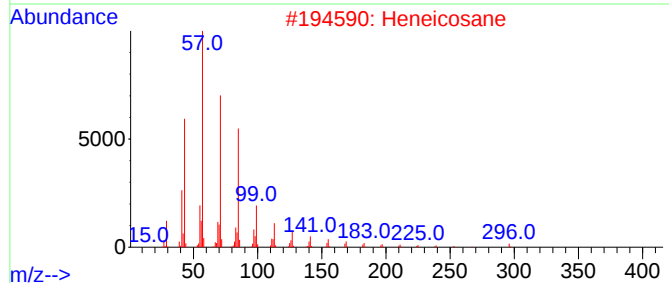
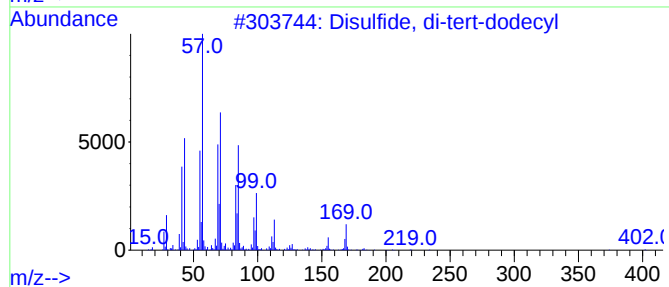
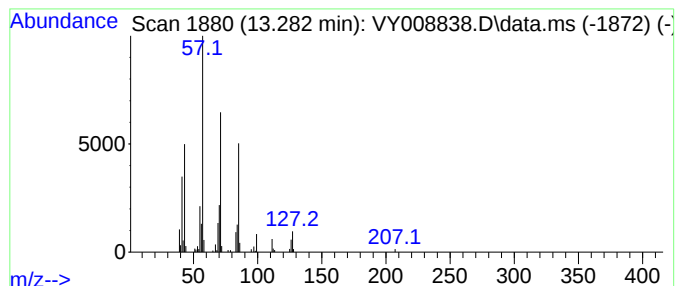
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051722S.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Disulfide, di-tert-dodecyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	5.70 ug/l	70310	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	72
2			Heneicosane	296	C21H44	000629-94-7	72
3			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
4			Pentacosane	352	C25H52	000629-99-2	59
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, di-t...	13.282	5.7	ug/l	70310	4	13.428	616515	50.0