

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
 Data File : VN073378.D
 Acq On : 07 Jul 2022 17:59
 Operator : JC\MD
 Sample : N3586-02
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31268

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_N\methods\82N062822W.M
 Title : SW846 8260

Signal : TIC: VN073378.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.381	77	84	87	rBV2	64378	136870	1.98%	0.166%
2	5.204	551	564	576	rBV	31639	124898	1.81%	0.152%
3	6.410	752	769	770	rBV	50373	144300	2.09%	0.175%
4	7.945	1018	1030	1034	rBV	189134	464483	6.72%	0.564%
5	8.004	1034	1040	1049	rVB	350484	834216	12.07%	1.013%
6	8.363	1089	1101	1113	rBV	197064	460053	6.66%	0.559%
7	8.745	1159	1166	1183	rBV3	34726	83806	1.21%	0.102%
8	8.892	1183	1191	1204	rVV	499481	1049059	15.18%	1.274%
9	9.381	1263	1274	1281	rBV2	50196	110574	1.60%	0.134%
10	10.375	1435	1443	1449	rBV	712023	1327074	19.20%	1.612%
11	10.439	1449	1454	1467	rVV	699174	1306574	18.91%	1.587%
12	11.469	1620	1629	1640	rVB4	46432	122176	1.77%	0.148%
13	11.569	1640	1646	1651	rBV2	41969	73828	1.07%	0.090%
14	11.686	1658	1666	1674	rBV	741977	1340451	19.40%	1.628%
15	11.780	1677	1682	1690	rBV	71581	127011	1.84%	0.154%
16	11.892	1690	1701	1711	rBV2	440525	872851	12.63%	1.060%
17	12.222	1744	1757	1764	rBV	205722	478027	6.92%	0.581%
18	12.304	1764	1771	1776	rVB	74857	123553	1.79%	0.150%
19	12.422	1788	1791	1802	rVB5	66349	152222	2.20%	0.185%
20	12.522	1802	1808	1811	rBV2	37613	77717	1.12%	0.094%
21	12.598	1812	1821	1823	rBV4	84476	157586	2.28%	0.191%
22	12.675	1828	1834	1839	rBV	608673	1022554	14.80%	1.242%
23	12.857	1857	1865	1869	rVB	88448	179929	2.60%	0.219%
24	12.922	1869	1876	1880	rBV	332948	594404	8.60%	0.722%
25	12.986	1880	1887	1894	rVV2	891351	1686884	24.41%	2.049%
26	13.045	1894	1897	1902	rVB3	80978	119949	1.74%	0.146%
27	13.163	1909	1917	1923	rBV2	164560	449337	6.50%	0.546%
28	13.222	1923	1927	1934	rVB	267995	418580	6.06%	0.508%
29	13.310	1934	1942	1947	rBV	666883	1137894	16.47%	1.382%
30	13.404	1954	1958	1961	rBV2	72703	117952	1.71%	0.143%
31	13.498	1967	1974	1979	rBV5	263777	531454	7.69%	0.646%
32	13.545	1979	1982	1985	rVV2	262313	389498	5.64%	0.473%
33	13.580	1985	1988	1989	rVV	174725	213184	3.09%	0.259%
34	13.610	1989	1993	2002	rVV2	1032577	2173528	31.45%	2.640%
35	13.680	2002	2005	2012	rVB	230455	332308	4.81%	0.404%
36	13.810	2022	2027	2030	rBV2	288787	408440	5.91%	0.496%

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37	13.851	2030	2034	2042	rVB3	248722	541171	7.83%	0.657%
38	13.933	2042	2048	2053	rBV	2201020	3198432	46.29%	3.885%
39	13.980	2053	2056	2058	rBV2	70249	81888	1.19%	0.099%
40	14.010	2058	2061	2064	rVB	71057	76725	1.11%	0.093%
41	14.098	2068	2076	2081	rBV3	340398	699000	10.12%	0.849%
42	14.151	2081	2085	2089	rBV	325502	459530	6.65%	0.558%
43	14.192	2089	2092	2098	rVB3	264537	431799	6.25%	0.525%
44	14.263	2098	2104	2109	rBV3	444382	749725	10.85%	0.911%
45	14.321	2109	2114	2120	rBV6	197548	401442	5.81%	0.488%
46	14.416	2121	2130	2132	rBV4	496426	1186245	17.17%	1.441%
47	14.445	2132	2135	2139	rVB4	458594	683179	9.89%	0.830%
48	14.486	2139	2142	2145	rBV	302430	355873	5.15%	0.432%
49	14.563	2151	2155	2156	rBV3	595580	794757	11.50%	0.965%
50	14.586	2156	2159	2167	rVB	1629814	2706736	39.17%	3.288%
51	14.663	2169	2172	2174	rBV3	119499	155004	2.24%	0.188%
52	14.698	2175	2178	2182	rVV	206109	260516	3.77%	0.316%
53	14.786	2182	2193	2198	rVV3	3117866	5198861	75.23%	6.316%
54	14.857	2199	2205	2210	rVV5	1036267	2577956	37.31%	3.132%
55	14.904	2210	2213	2221	rVB2	935242	1755170	25.40%	2.132%
56	15.021	2228	2233	2239	rVB	526618	990747	14.34%	1.204%
57	15.127	2247	2251	2255	rBV3	383952	552588	8.00%	0.671%
58	15.233	2263	2269	2275	rBV8	505911	1376695	19.92%	1.672%
59	15.321	2280	2284	2291	rVB5	700891	1372219	19.86%	1.667%
60	15.398	2291	2297	2302	rBV2	1163385	2385977	34.53%	2.898%
61	15.486	2309	2312	2317	rVB	262846	367044	5.31%	0.446%
62	15.539	2317	2321	2326	rBV2	487065	893678	12.93%	1.086%
63	15.627	2331	2336	2346	rVB	4014303	6910254	100.00%	8.395%
64	15.733	2346	2354	2361	rBV5	773432	2261834	32.73%	2.748%
65	15.810	2363	2367	2373	rVB2	560125	912809	13.21%	1.109%
66	15.939	2385	2389	2396	rVB	952594	1805670	26.13%	2.194%
67	16.098	2410	2416	2425	rBV7	566696	1791506	25.93%	2.176%
68	16.239	2434	2440	2448	rBV	2539900	6007195	86.93%	7.298%
69	16.315	2448	2453	2459	rVB6	715282	1510181	21.85%	1.835%
70	16.380	2459	2464	2470	rBV	829533	1455193	21.06%	1.768%
71	16.462	2472	2478	2484	rBV3	879934	1837197	26.59%	2.232%
72	16.521	2485	2488	2493	rVB4	352082	565576	8.18%	0.687%
73	16.592	2494	2500	2507	rBV	3710950	6859669	99.27%	8.333%
74	16.721	2517	2522	2525	rBV4	370453	804709	11.65%	0.978%

Sum of corrected areas: 82317974

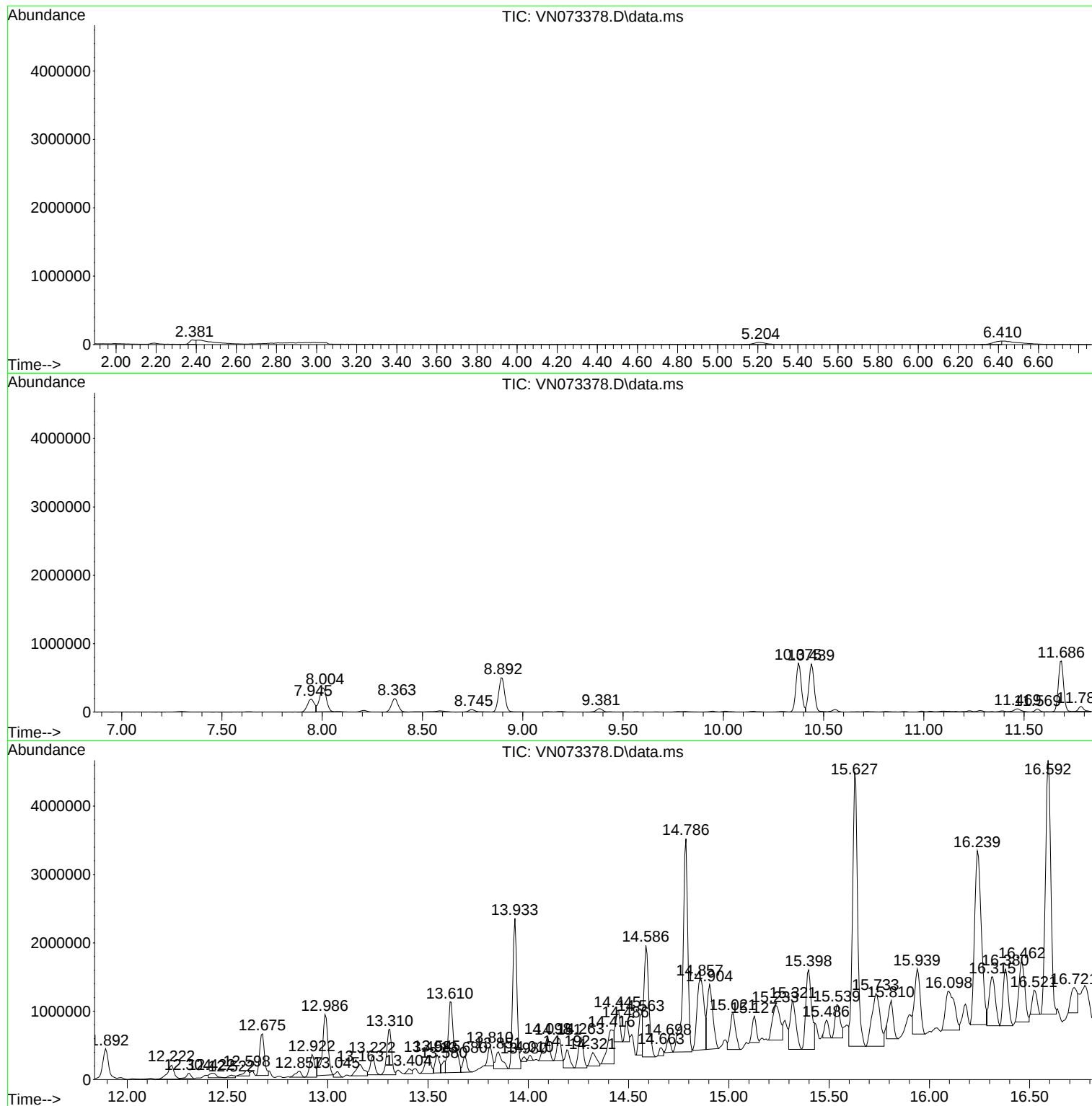
Instrument :
MSVOA_N
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31268

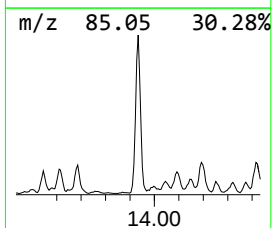
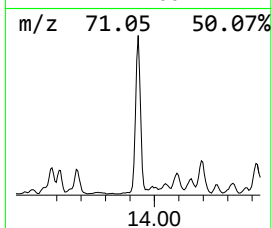
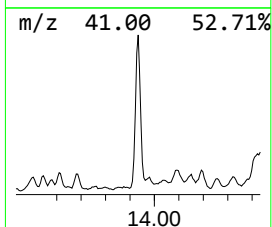
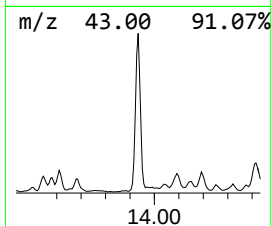
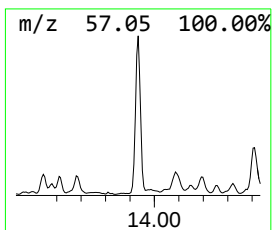
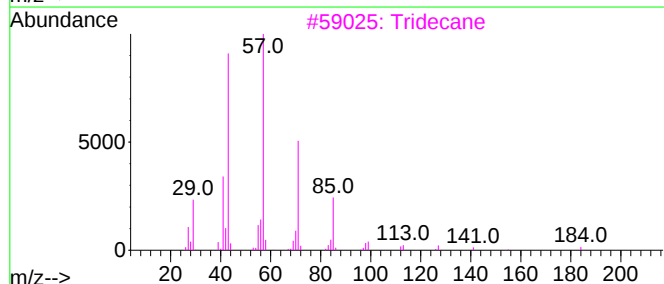
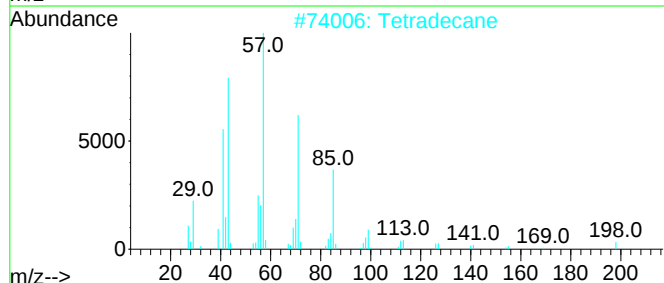
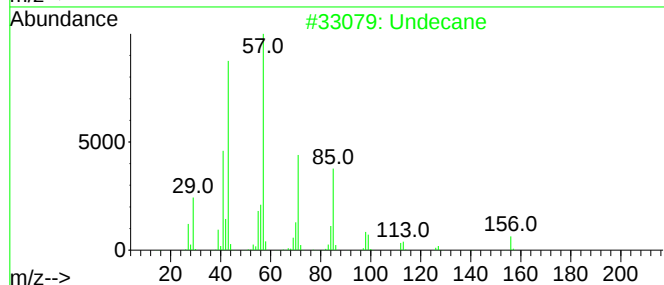
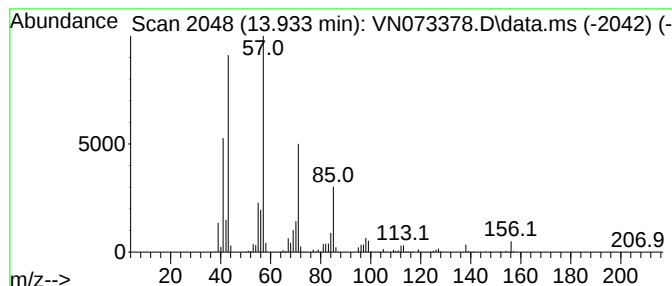
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	73.58 ug/l	3198430	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	92
2	Tetradecane			198	C14H30	000629-59-4	80
3	Tridecane			184	C13H28	000629-50-5	80
4	Decane			142	C10H22	000124-18-5	72
5	Octane, 2,4,6-trimethyl-			156	C11H24	062016-37-9	64



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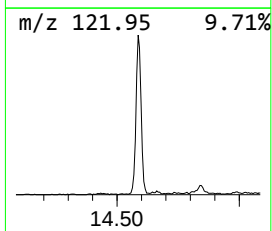
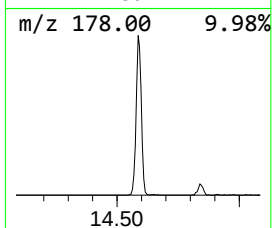
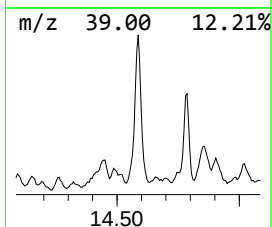
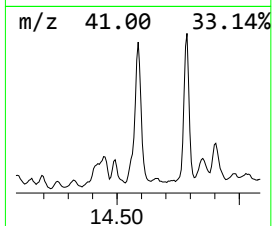
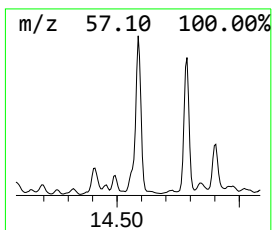
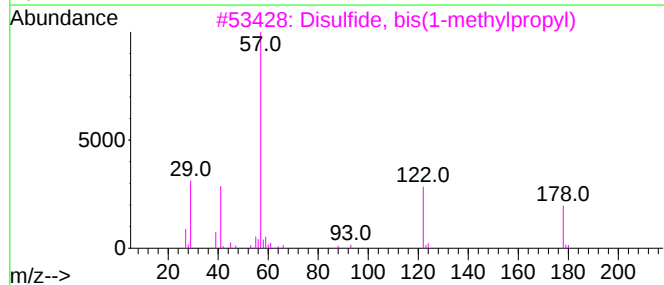
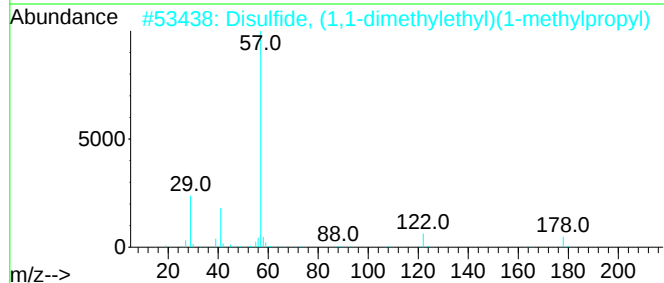
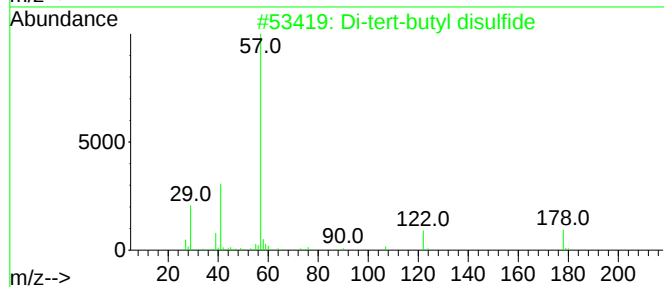
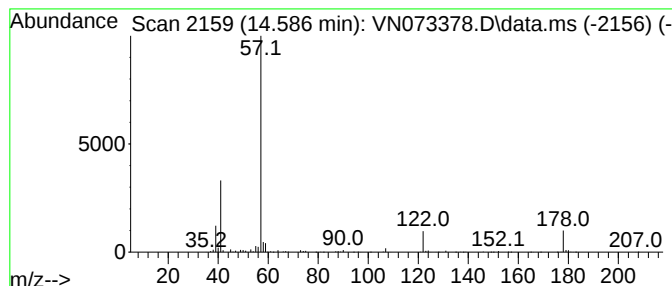
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 2 Di-tert-butyl disulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.586	62.27 ug/l	2706740	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	87
2			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	72
3			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	47
4			Disulfide, dibutyl	178	C8H18S2	000629-45-8	37
5			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	27



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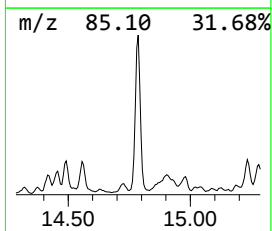
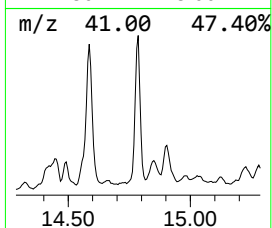
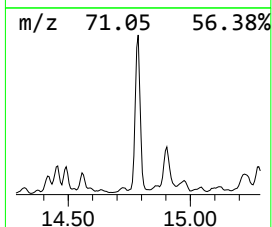
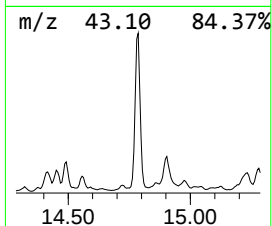
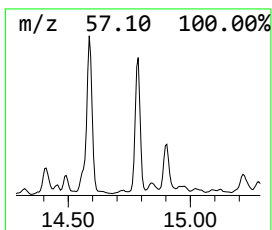
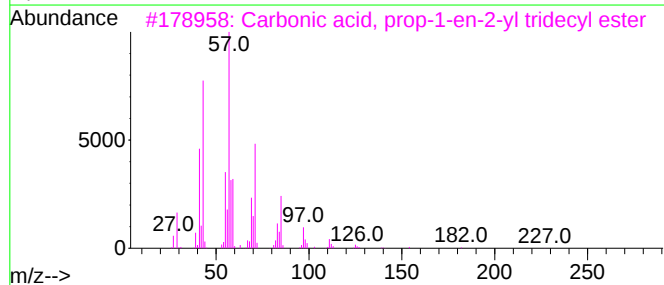
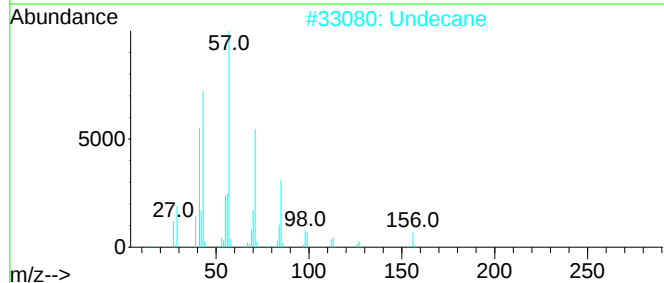
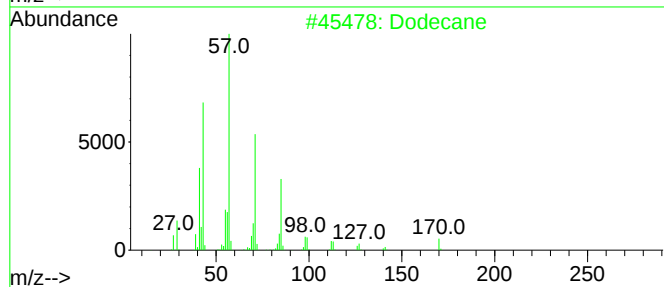
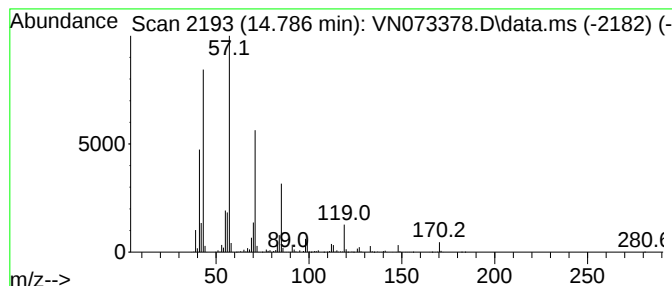
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

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

Peak Number 3 Dodecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.786	119.60 ug/l	5198860	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	95
2			Undecane	156	C11H24	001120-21-4	80
3			Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	80
4			Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	72
5			Tetradecane	198	C14H30	000629-59-4	72



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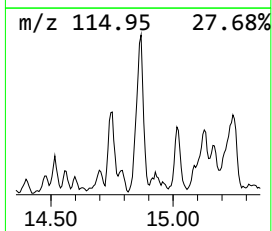
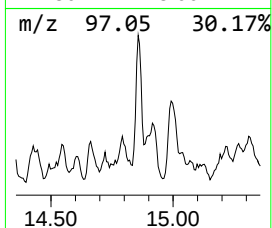
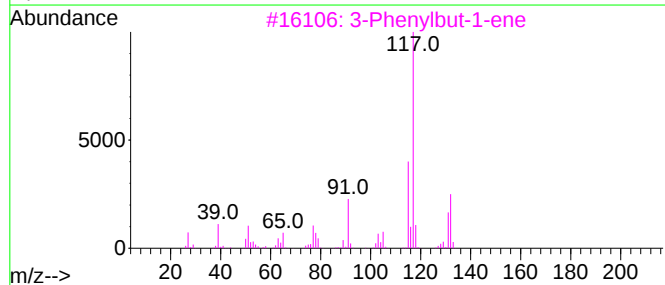
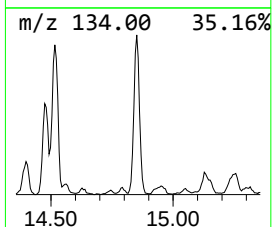
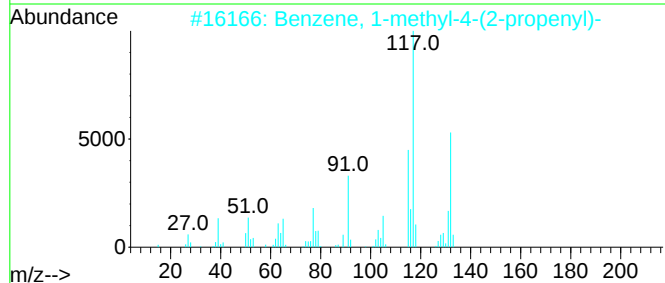
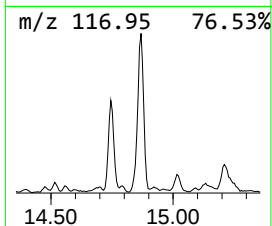
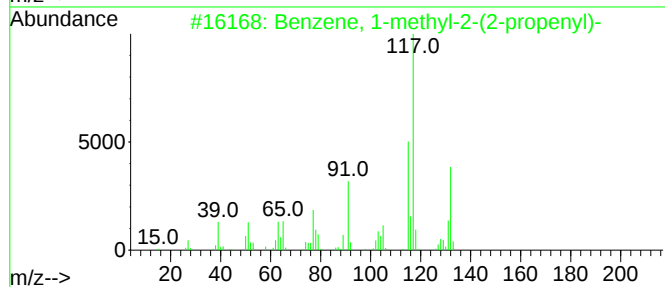
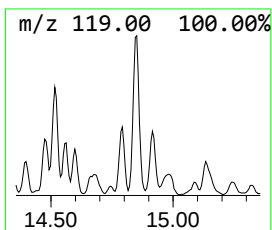
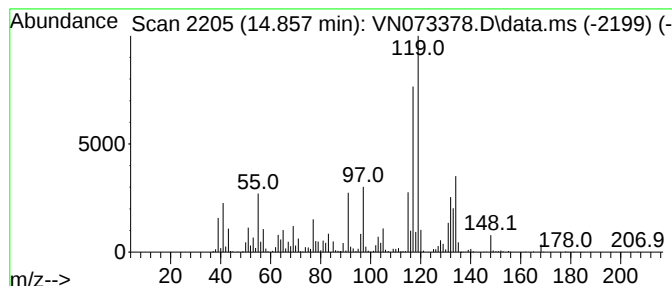
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1-methyl-2-(2-prop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	59.30 ug/l	2577960	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	94
2			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	89
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	86
4			Benzene, 2-butenyl-	132	C10H12	001560-06-1	86
5			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073378.D
Acq On : 07 Jul 2022 17:59
Operator : JC\MD
Sample : N3586-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31268

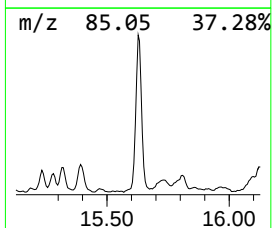
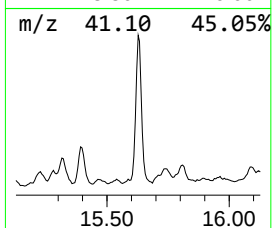
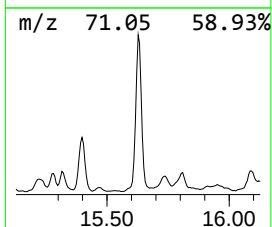
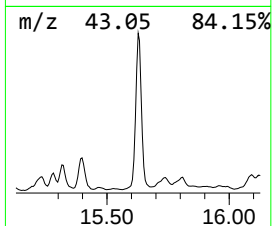
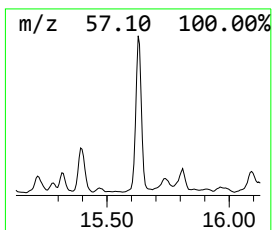
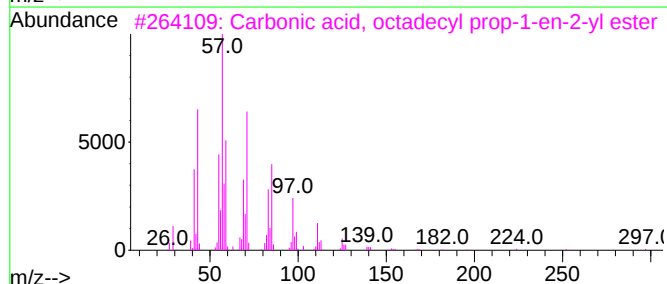
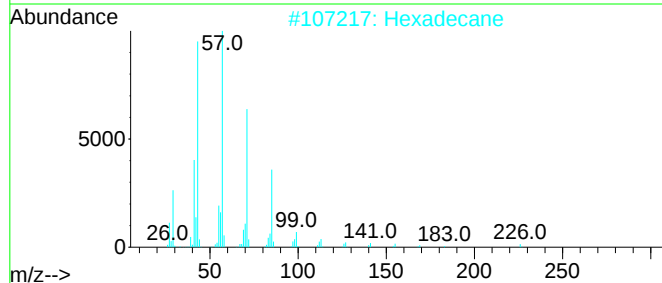
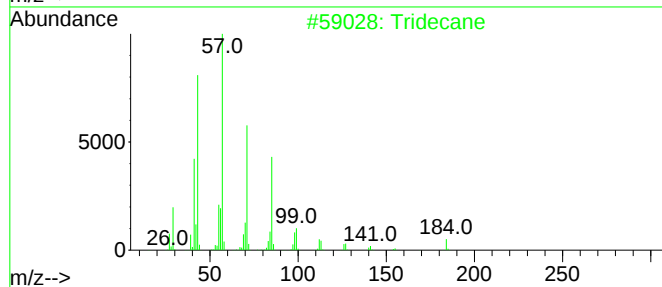
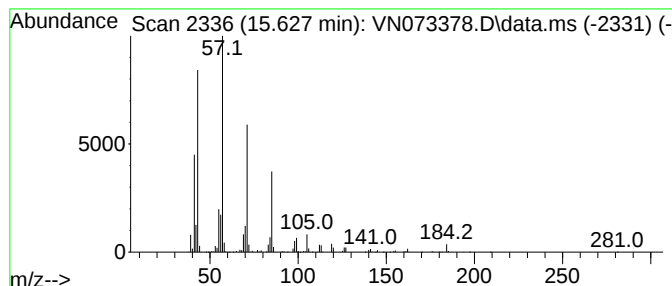
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Quant Title : SW846 8260

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

Peak Number 5 Tridecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.627	158.96 ug/l	6910250	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Hexadecane	226	C16H34	000544-76-3	83
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	80
4			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	72
5			Dodecane	170	C12H26	000112-40-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073378.D
Acq On : 07 Jul 2022 17:59
Operator : JC\MD
Sample : N3586-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31268

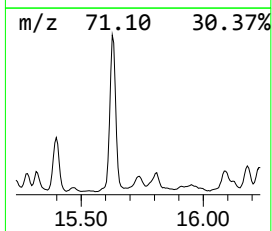
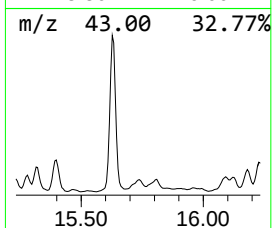
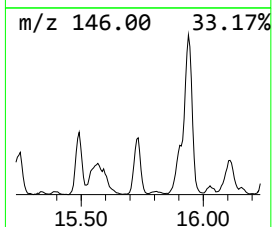
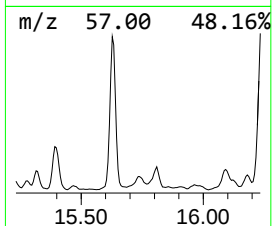
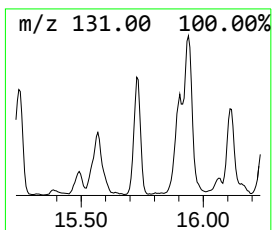
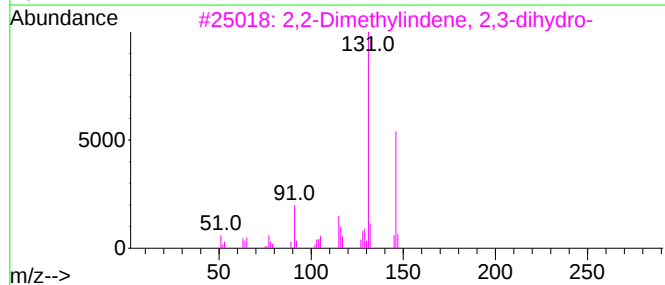
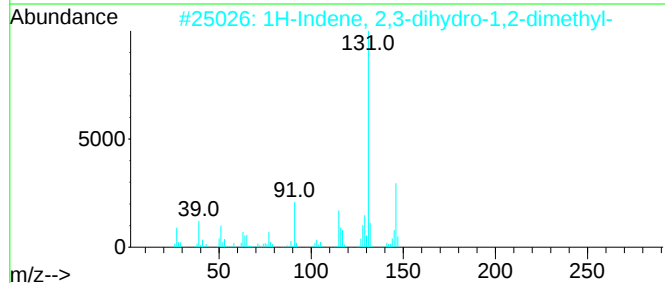
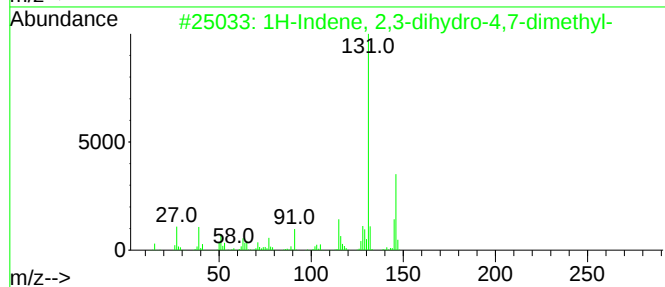
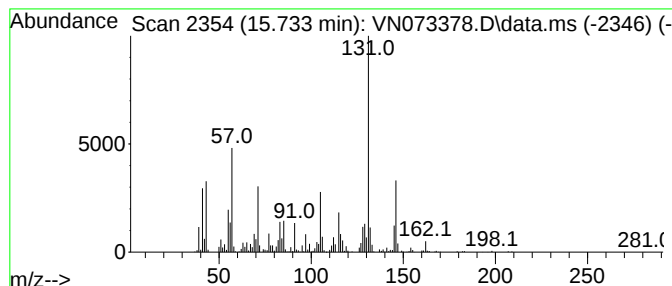
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Quant Title : SW846 8260

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

Peak Number 6 1H-Indene, 2,3-dihydro-4,7-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	52.03 ug/l	2261830	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	93
2			1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	86
3			2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	83
4			1H-Indene, 2,3-dihydro-1,6-dimet...	146	C11H14	017059-48-2	70
5			Benzene, 1-methyl-4-(1-methyl-2-...	146	C11H14	097664-18-1	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073378.D
Acq On : 07 Jul 2022 17:59
Operator : JC\MD
Sample : N3586-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

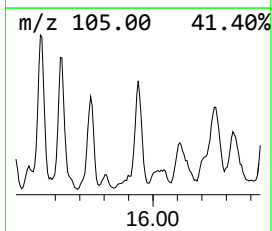
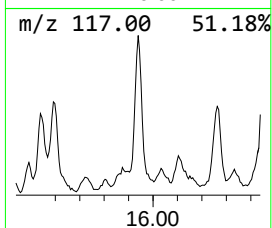
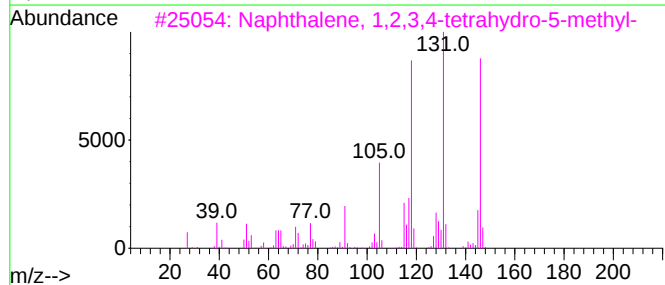
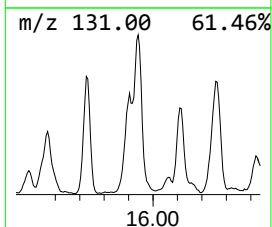
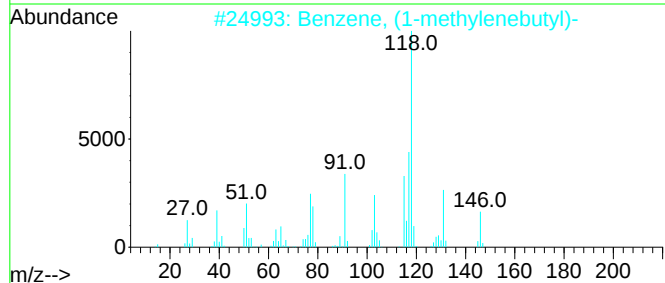
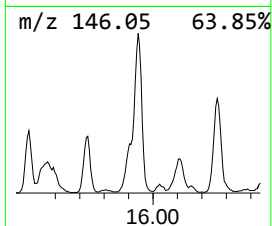
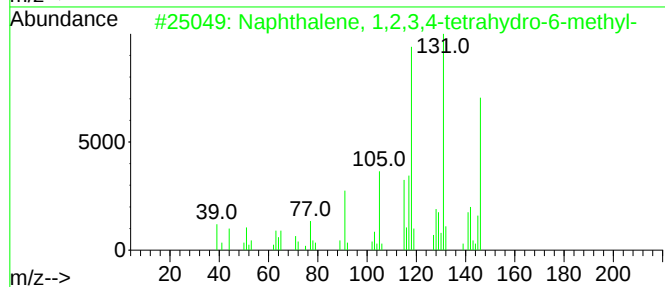
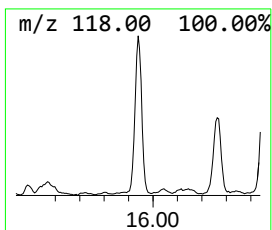
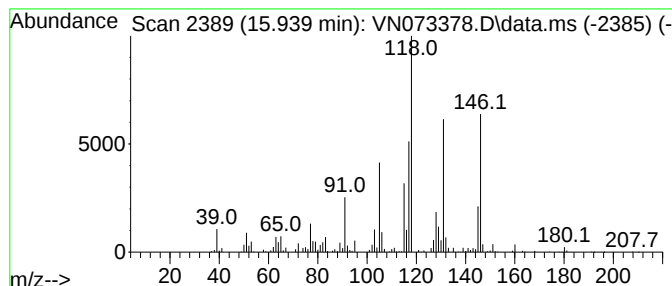
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MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 1,2,3,4-tetrahydro-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.939	41.54 ug/l	1805670	1,4-Dichlorobenzene-d4		13.616	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	001680-51-9	91
2	Benzene, (1-methylenebutyl)-		146	C11H14	005676-32-4	87
3	Naphthalene, 1,2,3,4-tetrahydro-...		146	C11H14	002809-64-5	83
4	Naphthalene, 1,2,3,4-tetrahydro-...		160	C12H16	004175-54-6	70
5	2,3,4,5,6,7-Hexahydro-1H-cyclope...		146	C11H14	1010189-31-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073378.D
Acq On : 07 Jul 2022 17:59
Operator : JC\MD
Sample : N3586-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31268

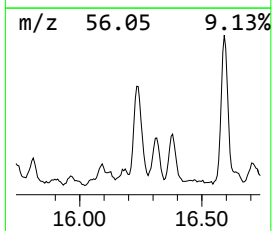
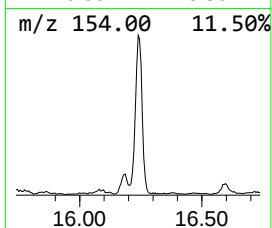
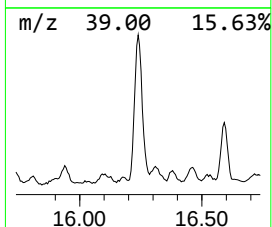
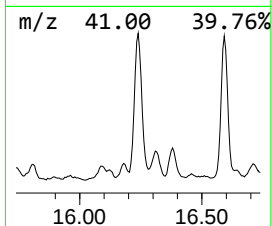
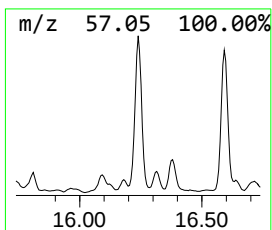
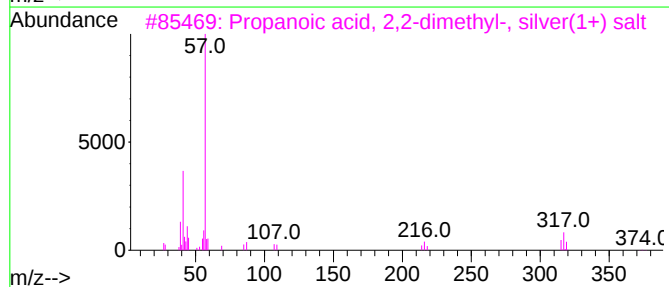
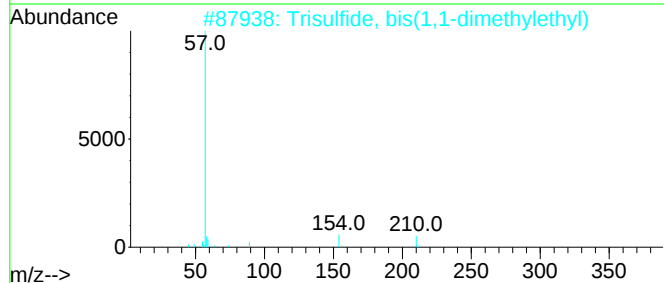
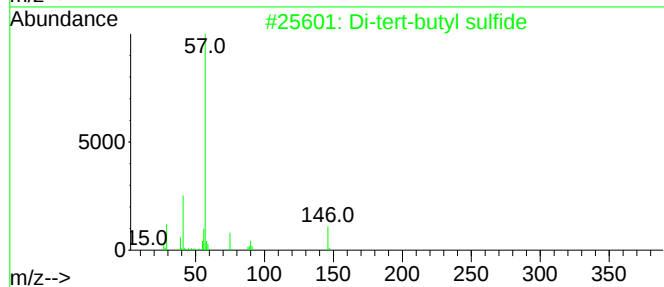
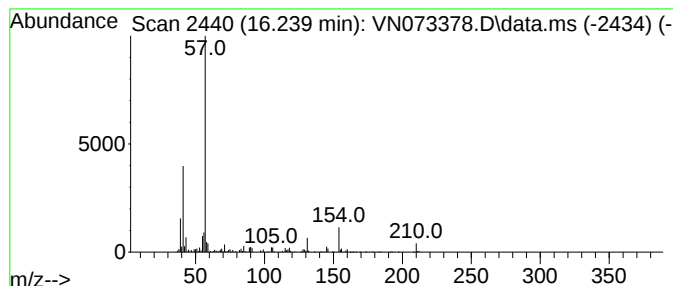
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Quant Title : SW846 8260

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

Peak Number 8 unknown16.239 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.239	138.19 ug/l	6007200	1,4-Dichlorobenzene-d4	13.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Di-tert-butyl sulfide	146	C8H18S	000107-47-1	43
2		Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	38
3		Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	38
4		Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	35
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073378.D
Acq On : 07 Jul 2022 17:59
Operator : JC\MD
Sample : N3586-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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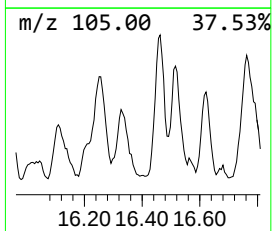
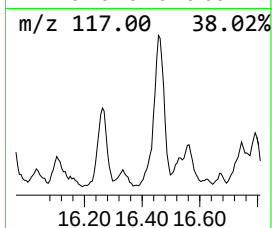
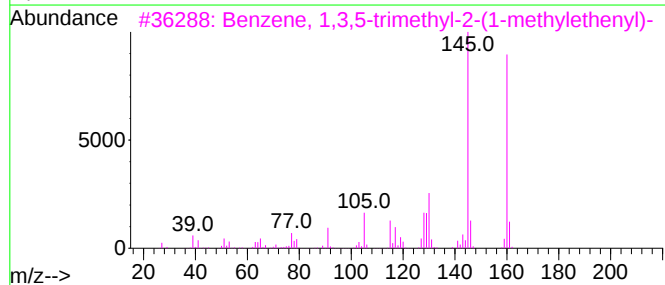
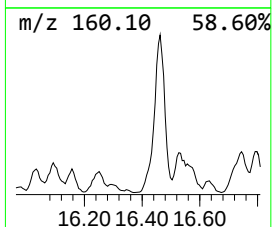
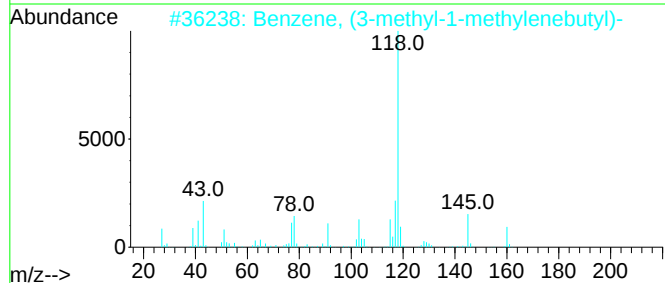
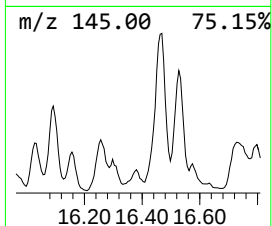
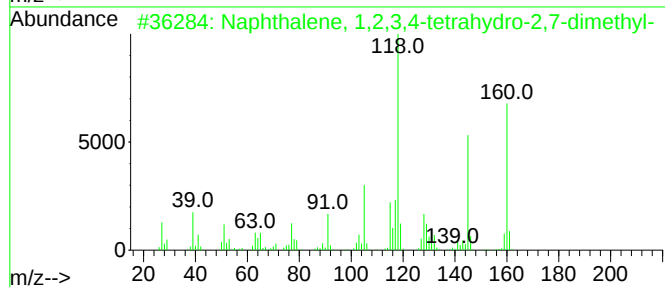
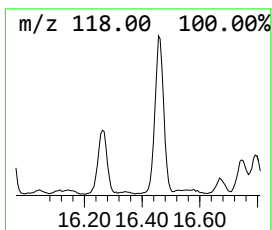
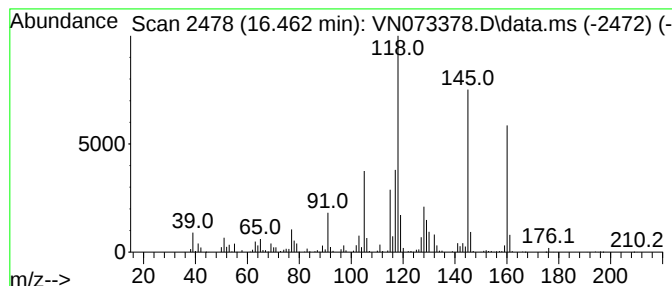
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1,2,3,4-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	42.26 ug/l	1837200	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	81
2			Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	74
3			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	70
4			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	64
5			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073378.D
Acq On : 07 Jul 2022 17:59
Operator : JC\MD
Sample : N3586-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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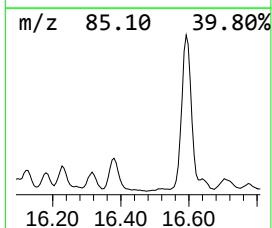
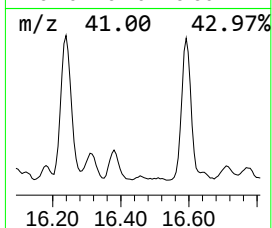
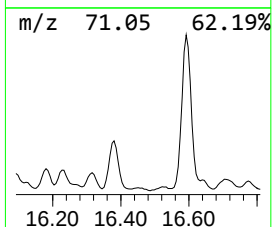
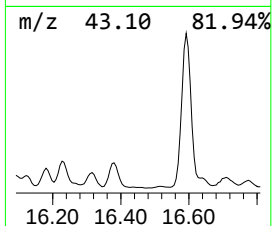
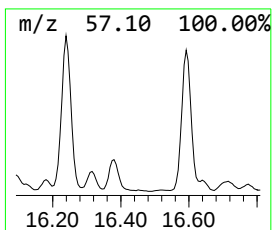
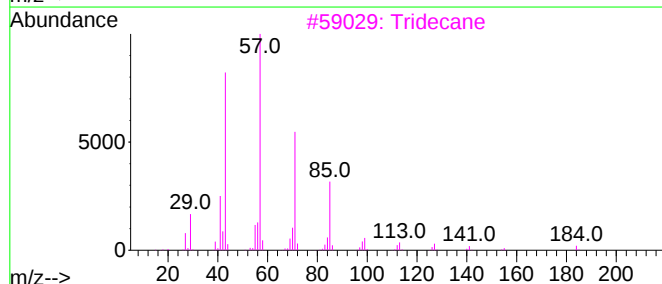
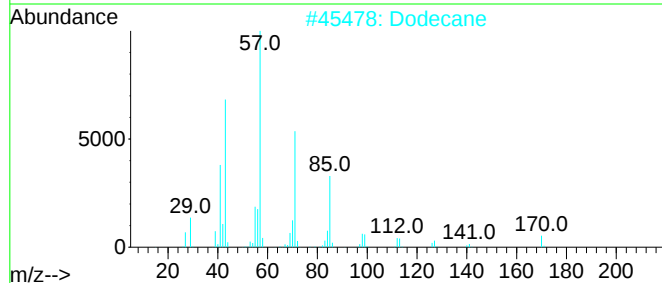
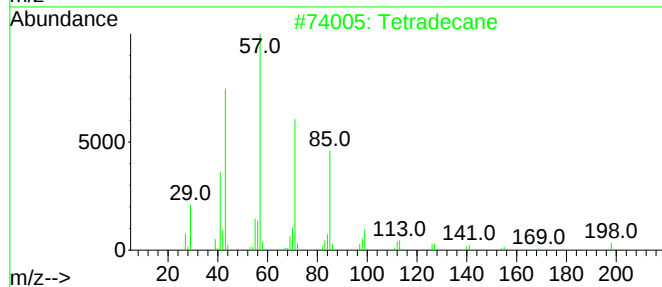
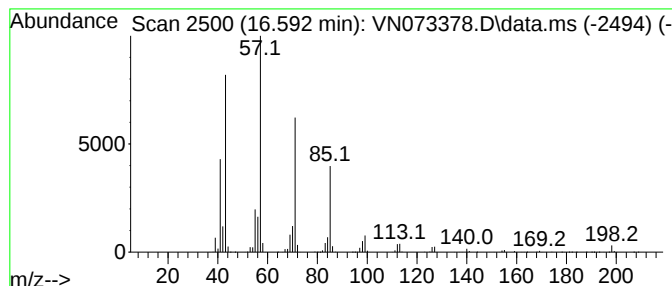
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Quant Title : SW846 8260

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

Peak Number 10 Tetradecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.592	157.80 ug/l	6859670	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	97
2			Dodecane	170	C12H26	000112-40-3	90
3			Tridecane	184	C13H28	000629-50-5	90
4			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	86
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN070722\
Data File : VN073378.D
Acq On : 07 Jul 2022 17:59
Operator : JC\MD
Sample : N3586-02
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31268

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecane	13.933	73.6	ug/l	3198430	4	13.616	2173530	50.0
Di-tert-butyl d...	14.586	62.3	ug/l	2706740	4	13.616	2173530	50.0
Dodecane	14.786	119.6	ug/l	5198860	4	13.616	2173530	50.0
Benzene, 1-meth...	14.857	59.3	ug/l	2577960	4	13.616	2173530	50.0
Tridecane	15.627	159.0	ug/l	6910250	4	13.616	2173530	50.0
1H-Indene, 2,3-...	15.733	52.0	ug/l	2261830	4	13.616	2173530	50.0
Naphthalene, 1,...	15.939	41.5	ug/l	1805670	4	13.616	2173530	50.0
unknown16.239	16.239	138.2	ug/l	6007200	4	13.616	2173530	50.0
Naphthalene, 1,...	16.462	42.3	ug/l	1837200	4	13.616	2173530	50.0
Tetradecane	16.592	157.8	ug/l	6859670	4	13.616	2173530	50.0