

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
 Data File : VN067541.D
 Acq On : 28 Jun 2021 19:29
 Operator : JC/MD
 Sample : M2802-02
 Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41817

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\82N062821W.M
 Title : SW846 8260

Signal : TIC: VN067541.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.021	2226	2249	2256	rBV2	163955	395257	10.40%	2.818%
2	8.078	2261	2270	2289	rVV	322739	754784	19.86%	5.382%
3	8.161	2290	2301	2323	rVB4	40048	96264	2.53%	0.686%
4	8.284	2327	2347	2367	rBV3	120151	275478	7.25%	1.964%
5	8.434	2382	2403	2427	rBV	185585	425117	11.19%	3.031%
6	8.547	2428	2445	2463	rVV5	20842	54319	1.43%	0.387%
7	8.818	2529	2546	2570	rBV2	76343	151992	4.00%	1.084%
8	8.965	2579	2601	2642	rBV	434168	931189	24.51%	6.640%
9	9.451	2757	2782	2796	rBV4	34841	86172	2.27%	0.614%
10	10.443	3133	3152	3163	rBV	710561	1337392	35.20%	9.536%
11	10.507	3163	3176	3209	rVB	1998949	3799930	100.00%	27.094%
12	11.749	3621	3639	3666	rBV	606621	1117358	29.40%	7.967%
13	11.956	3694	3716	3737	rBV5	53468	107776	2.84%	0.768%
14	12.371	3855	3871	3881	rBV3	26017	43175	1.14%	0.308%
15	12.487	3892	3914	3928	rBV3	24359	68869	1.81%	0.491%
16	12.736	3994	4007	4030	rVB	480091	854020	22.47%	6.089%
17	12.902	4059	4069	4085	rVB6	21469	49824	1.31%	0.355%
18	12.986	4085	4100	4108	rBV5	34916	66853	1.76%	0.477%
19	13.050	4111	4124	4140	rVB	220134	388752	10.23%	2.772%
20	13.286	4203	4212	4227	rVB2	66682	102967	2.71%	0.734%
21	13.372	4233	4244	4254	rBV	59379	98150	2.58%	0.700%
22	13.562	4303	4315	4325	rBV10	50281	107872	2.84%	0.769%
23	13.611	4327	4333	4341	rVV5	37647	56769	1.49%	0.405%
24	13.678	4345	4358	4377	rVB	602555	1056146	27.79%	7.531%
25	13.994	4466	4476	4489	rBV	211298	325983	8.58%	2.324%
26	14.324	4589	4599	4610	rBV7	21918	38185	1.00%	0.272%
27	14.651	4703	4721	4740	rVB	171461	334513	8.80%	2.385%
28	14.847	4787	4794	4806	rVB	102779	152393	4.01%	1.087%
29	14.917	4809	4820	4831	rBV6	40082	81926	2.16%	0.584%
30	15.469	5017	5026	5034	rBV3	25698	45101	1.19%	0.322%
31	15.702	5103	5113	5133	rVB	92261	162433	4.27%	1.158%
32	16.327	5331	5346	5363	rBV3	192243	409229	10.77%	2.918%
33	16.681	5472	5478	5489	rVB3	31206	48646	1.28%	0.347%

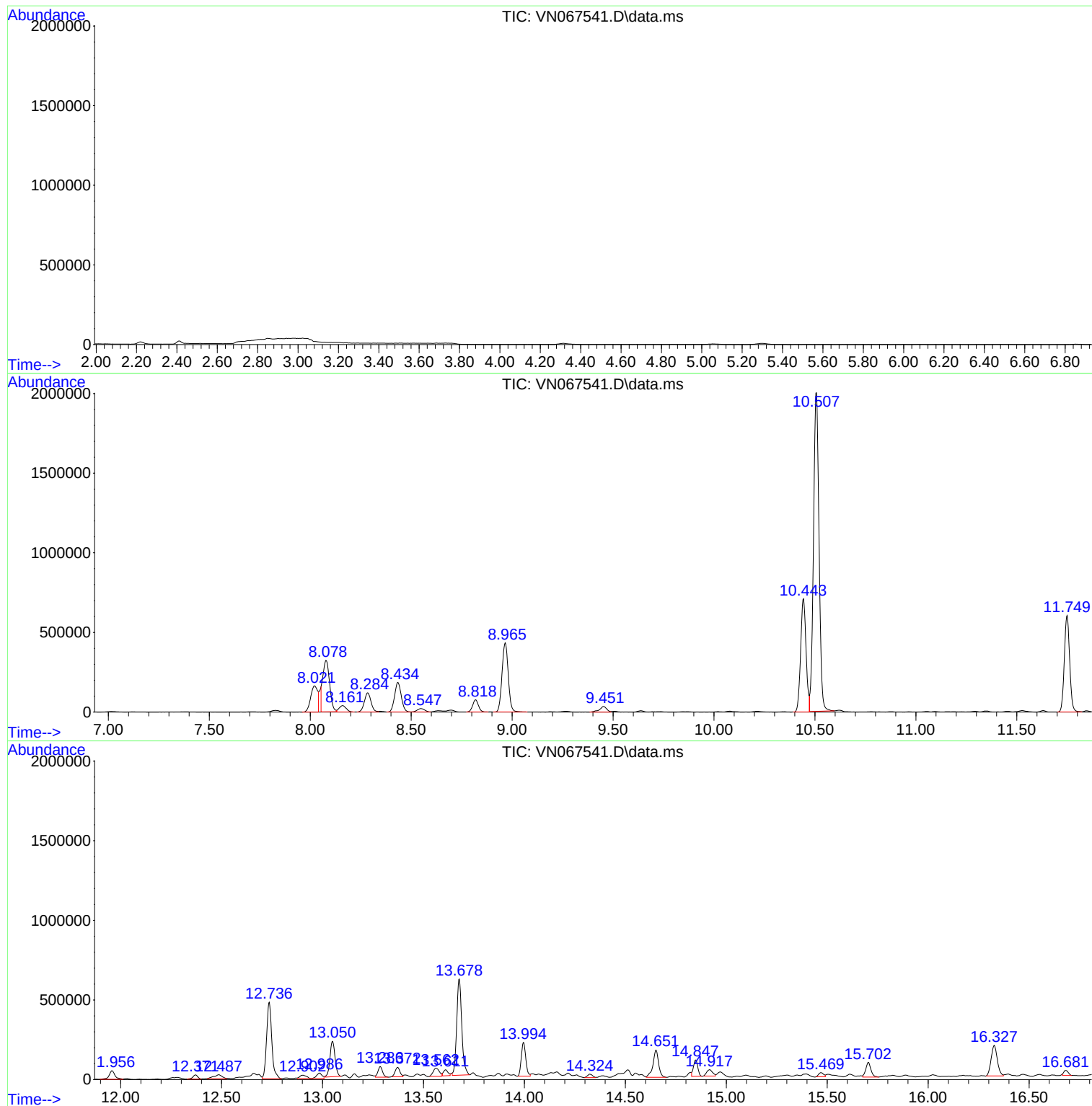
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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



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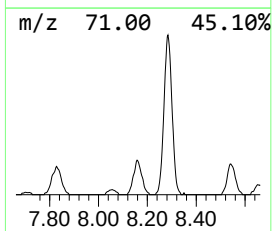
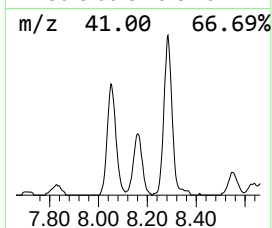
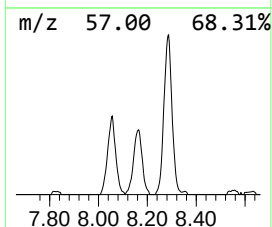
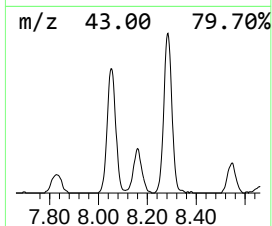
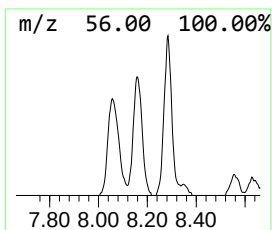
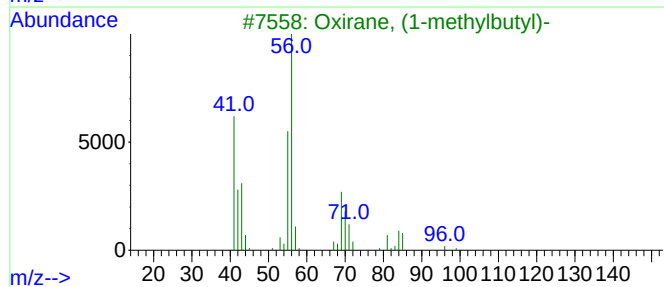
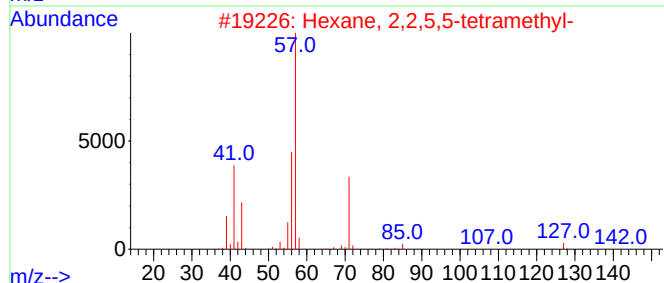
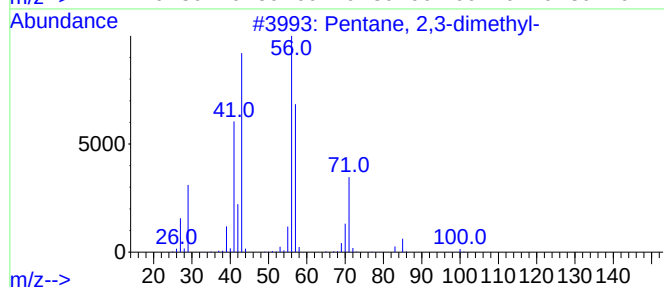
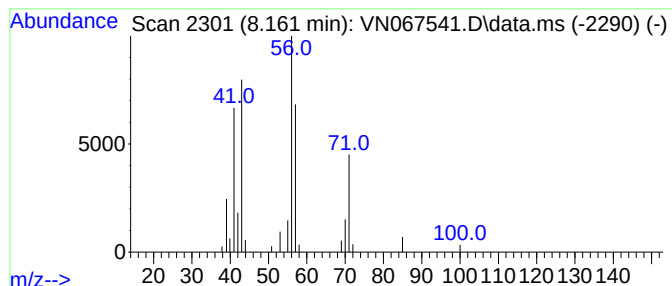
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.161	6.38 ug/l	96264	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	72
3			Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	53
4			Heptane	100	C7H16	000142-82-5	47
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	46



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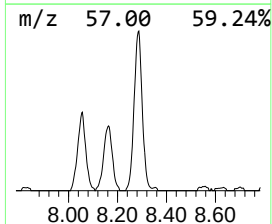
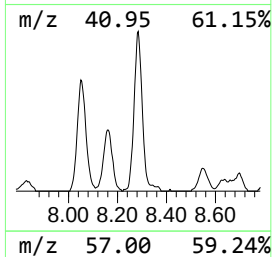
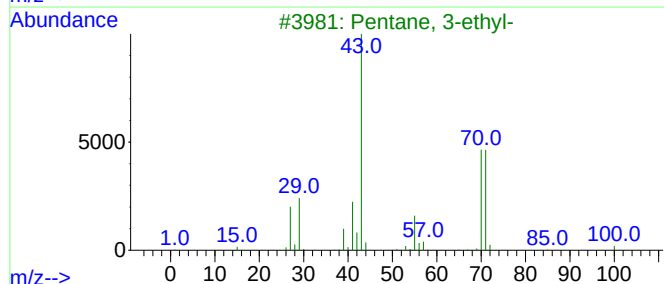
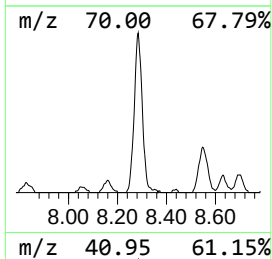
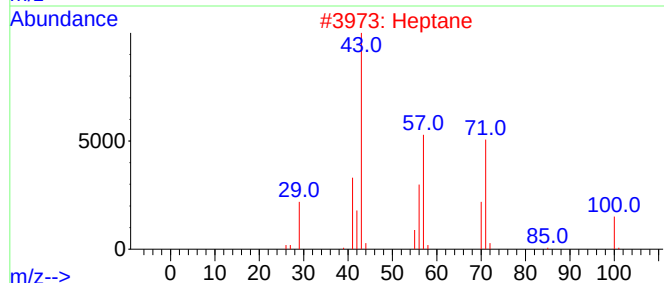
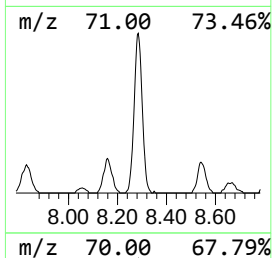
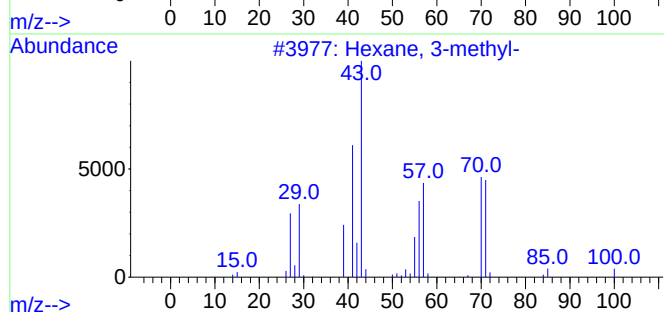
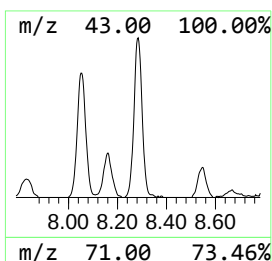
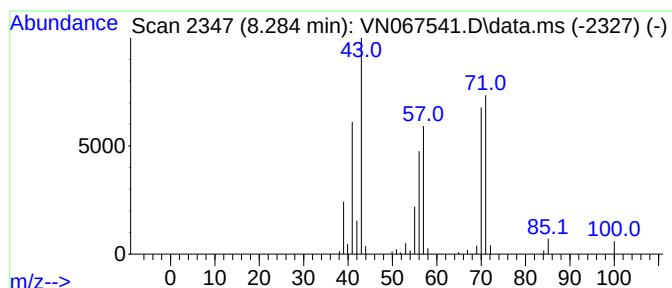
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.284	18.25 ug/l	275478	Pentafluorobenzene	8.080

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2		Heptane	100	C7H16	000142-82-5	80
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	59
4		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	59
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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ALS Vial : 20 Sample Multiplier: 1

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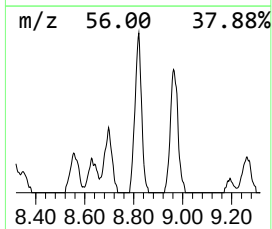
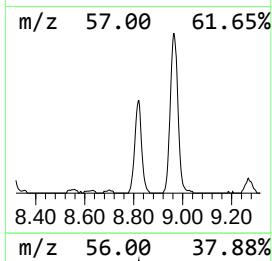
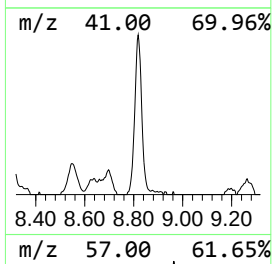
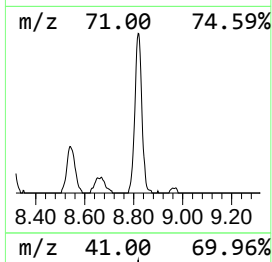
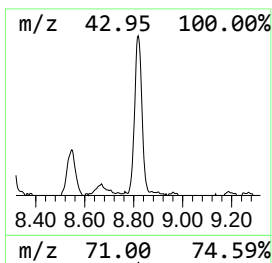
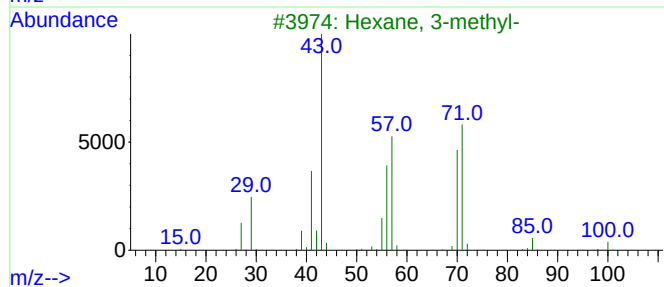
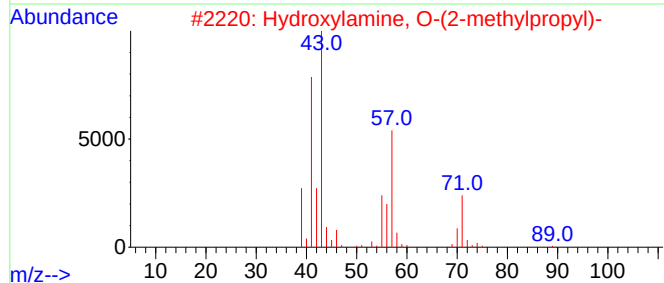
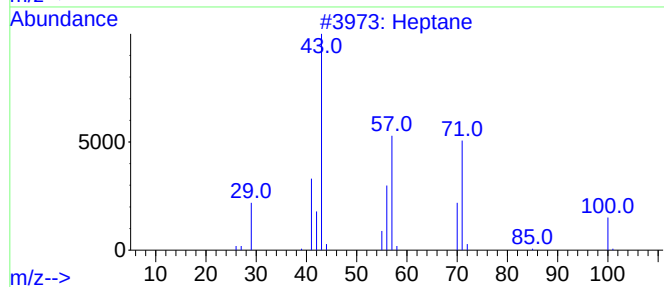
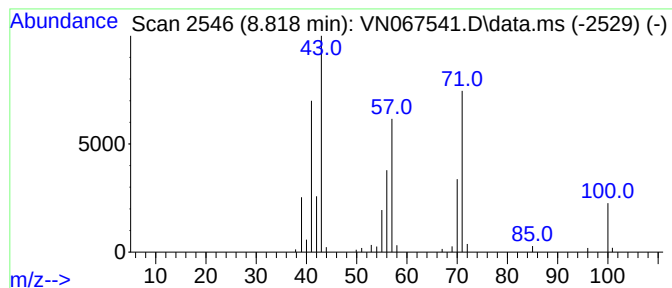
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.818	8.16 ug/l	151992	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	80
2			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	72
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
4			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
5			Oxirane, butyl-	100	C6H12O	001436-34-6	43



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ALS Vial : 20 Sample Multiplier: 1

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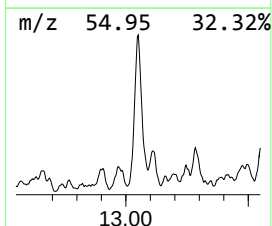
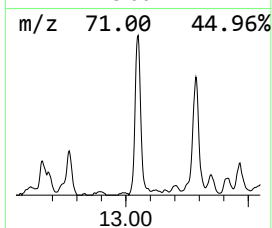
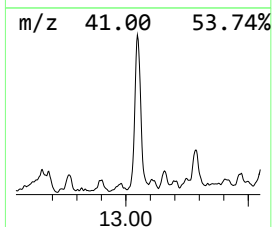
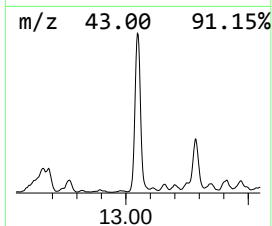
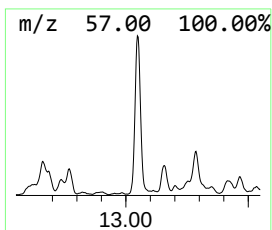
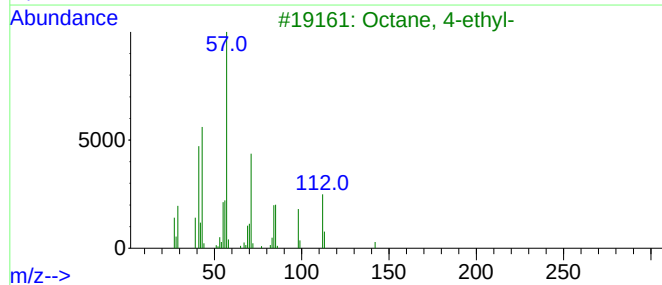
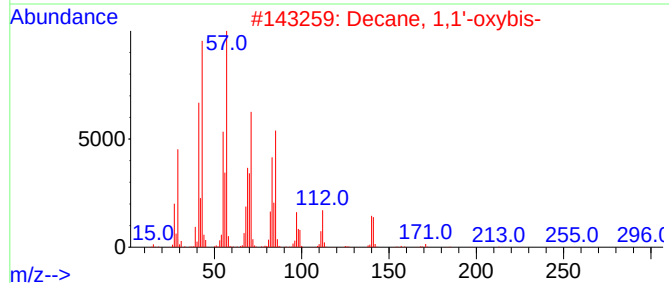
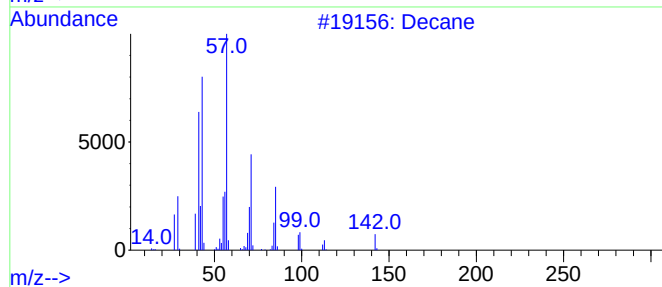
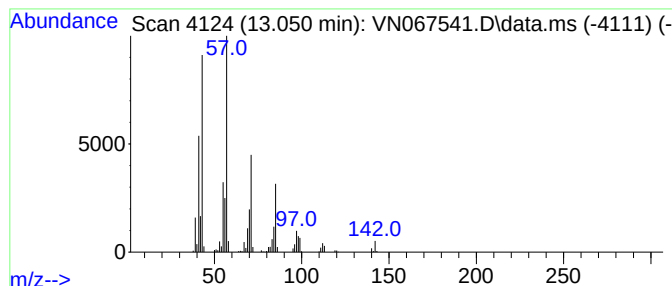
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.050	18.40 ug/l	388752	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	93
2			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	72
3			Octane, 4-ethyl-	142	C10H22	015869-86-0	64
4			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	59
5			1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59



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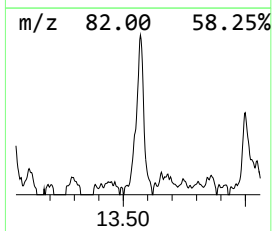
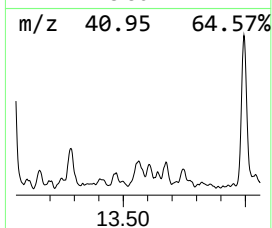
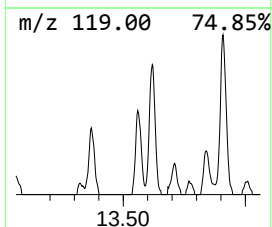
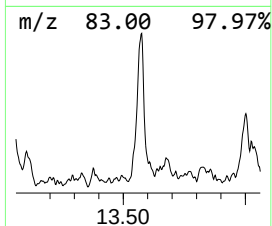
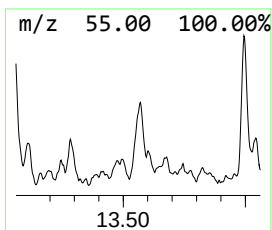
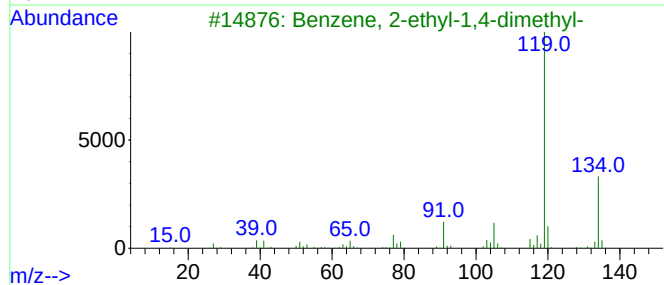
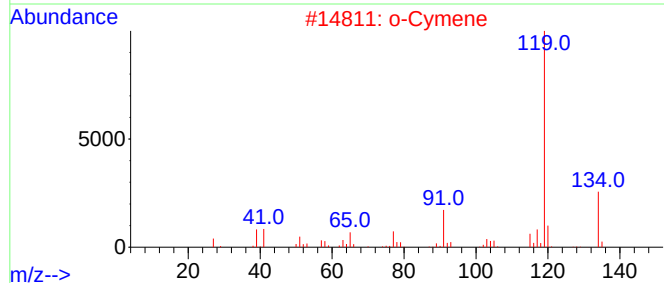
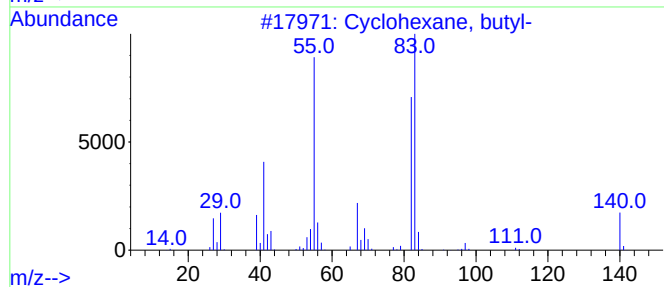
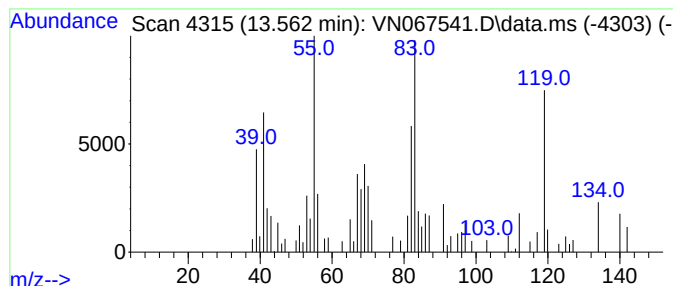
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

Peak Number 5 unknown13.562 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.562	5.11 ug/l	107872	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, butyl-	140	C10H20	001678-93-9	38
2			o-Cymene	134	C10H14	000527-84-4	30
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	30
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	30
5			p-Cymene	134	C10H14	000099-87-6	30



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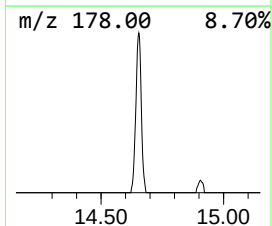
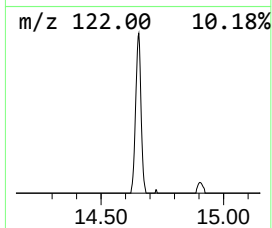
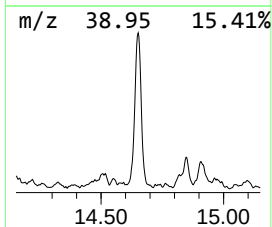
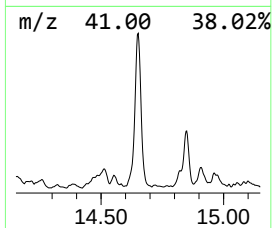
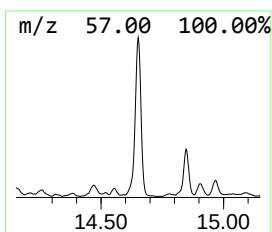
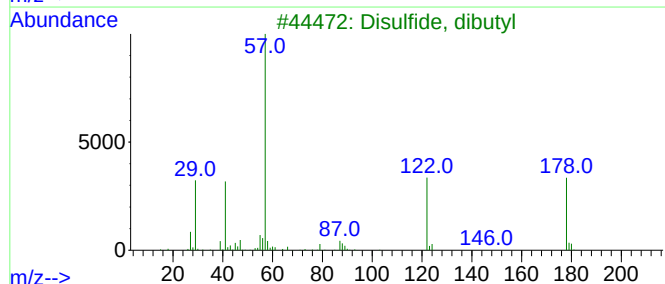
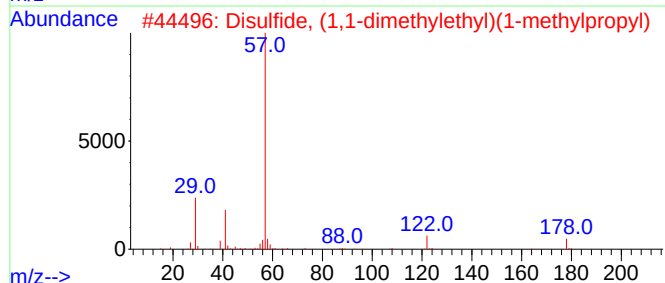
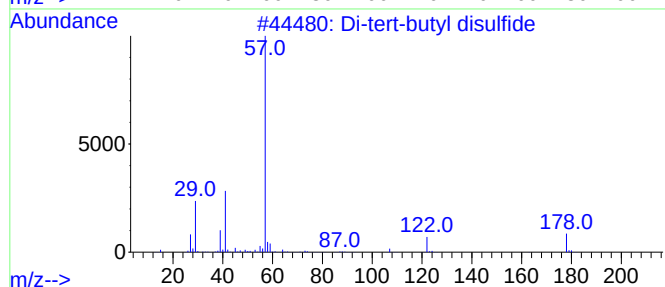
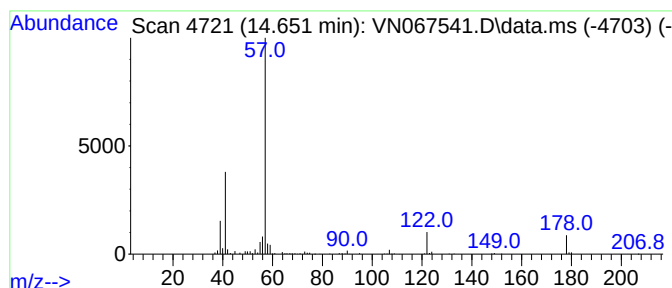
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Quant Title : SW846 8260

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

Peak Number 6 Di-tert-butyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	15.84 ug/l	334513	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	80
2			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	64
3			Disulfide, dibutyl	178	C8H18S2	000629-45-8	52
4			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	37
5			Butane, 2-bromo-	136	C4H9Br	000078-76-2	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067541.D
Acq On : 28 Jun 2021 19:29
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

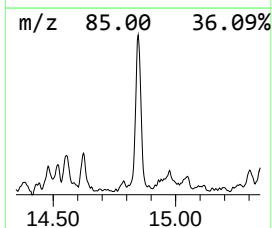
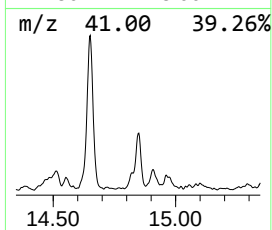
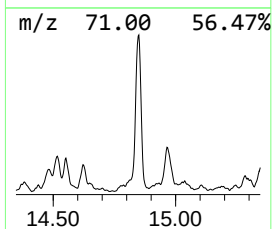
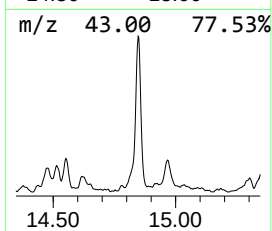
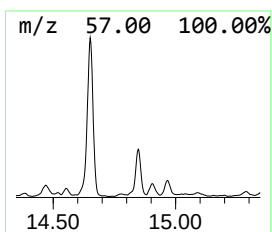
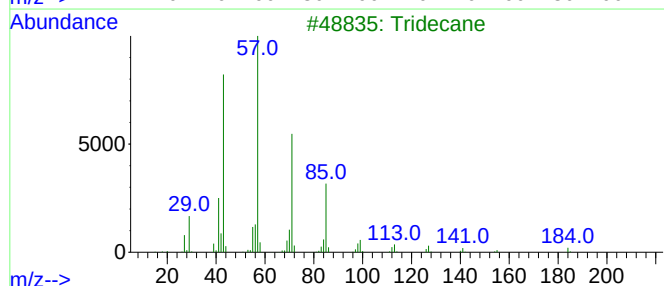
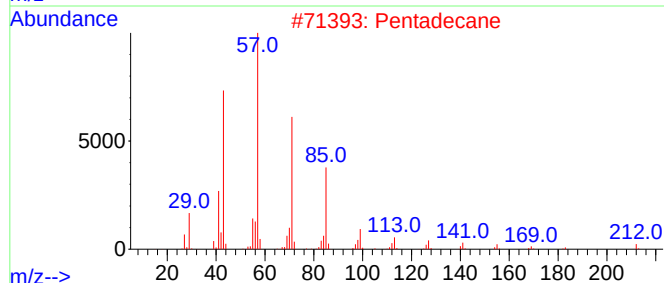
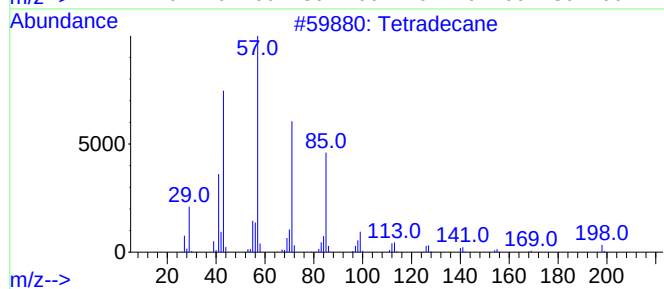
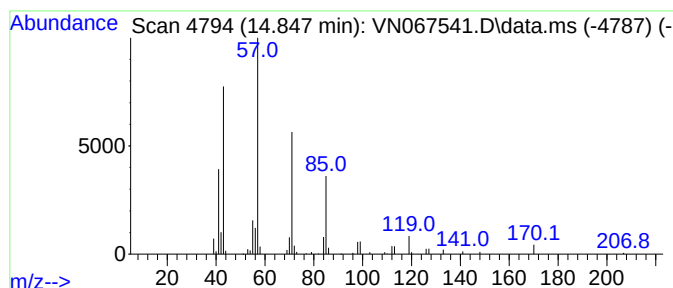
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Quant Title : SW846 8260

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

Peak Number 7 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.847	7.21 ug/l	152393	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	86
2			Pentadecane	212	C15H32	000629-62-9	80
3			Tridecane	184	C13H28	000629-50-5	78
4			Hexadecane	226	C16H34	000544-76-3	72
5			Dodecane	170	C12H26	000112-40-3	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067541.D
Acq On : 28 Jun 2021 19:29
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

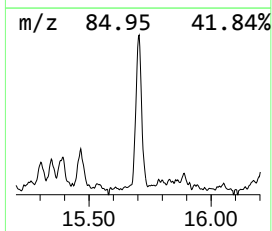
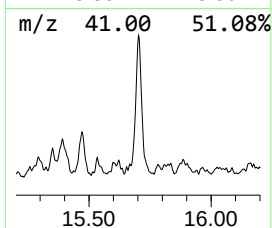
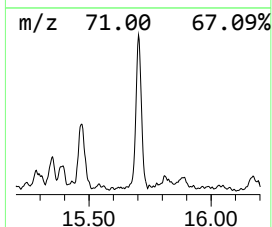
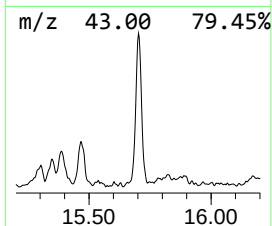
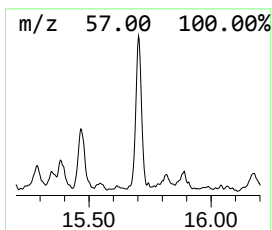
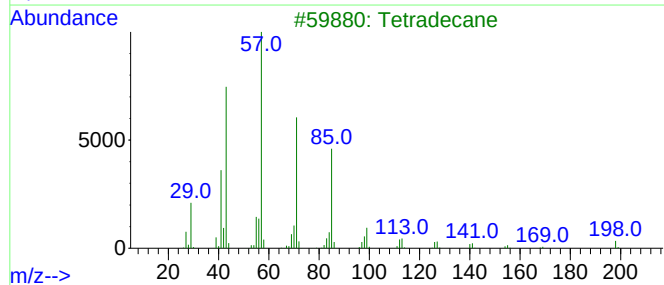
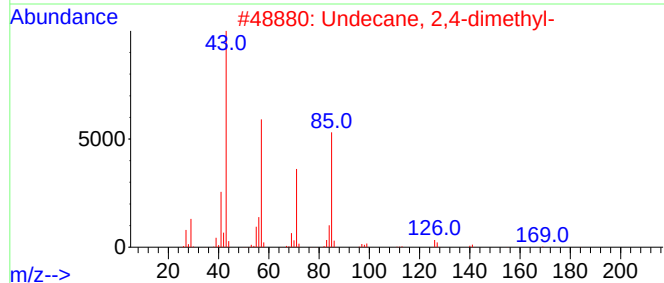
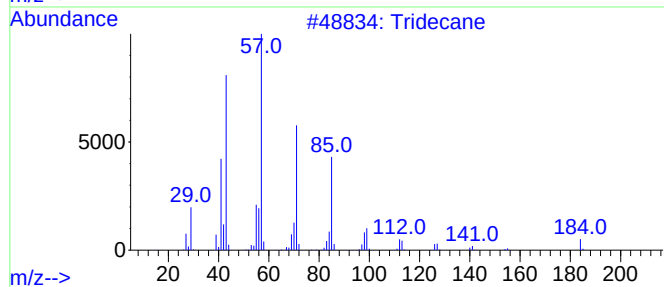
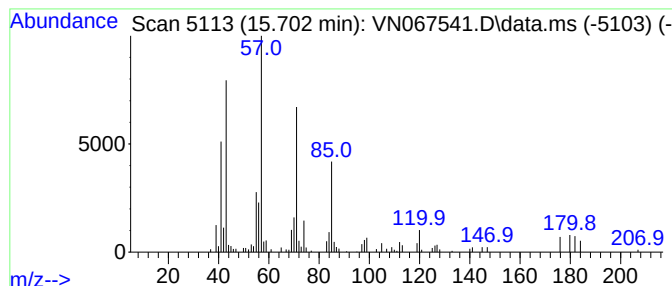
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Quant Title : SW846 8260

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

Peak Number 8 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.702	7.69 ug/l	162433	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	93
2			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	64
3			Tetradecane	198	C14H30	000629-59-4	64
4			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	64
5			Nonane	128	C9H20	000111-84-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067541.D
Acq On : 28 Jun 2021 19:29
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

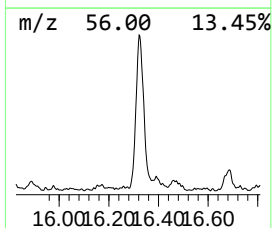
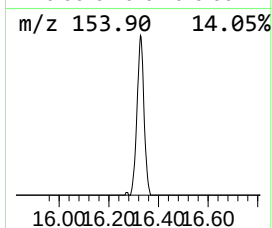
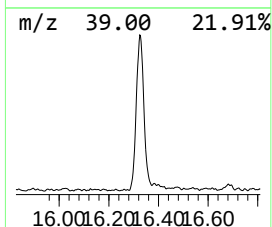
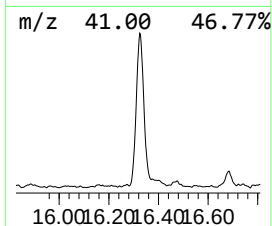
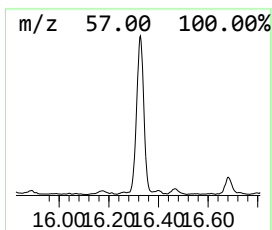
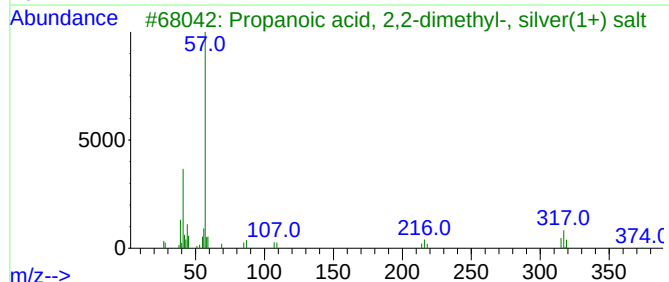
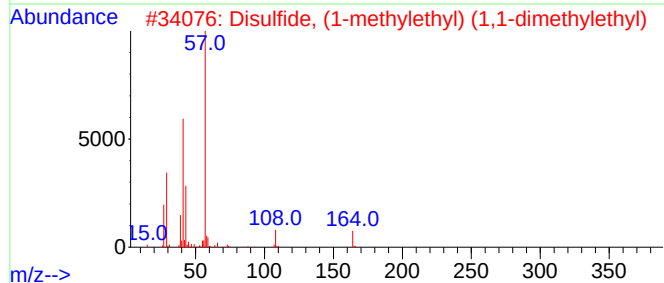
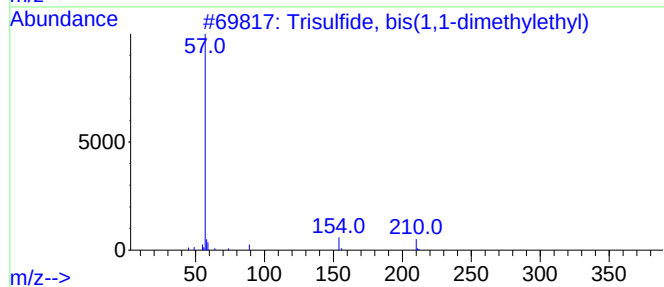
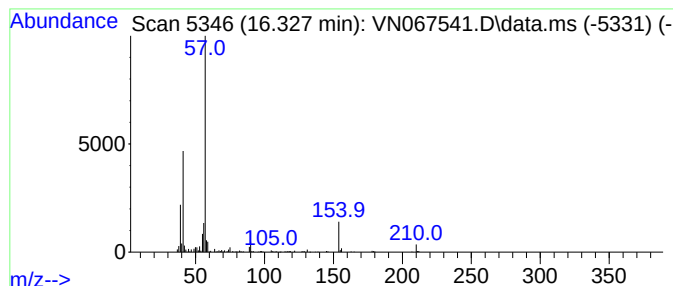
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

Peak Number 9 Trisulfide, bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.327	19.37 ug/l	409229	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	59
2			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	32
3			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	32
4			Butane, 2-bromo-	136	C4H9Br	000078-76-2	25
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062821\
Data File : VN067541.D
Acq On : 28 Jun 2021 19:29
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N062821W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,3-di...	8.161	6.4	ug/l	96264	1	8.080	754784	50.0
Hexane, 3-methyl-	8.284	18.3	ug/l	275478	1	8.080	754784	50.0
Heptane	8.818	8.2	ug/l	151992	2	8.965	931189	50.0
Decane	13.050	18.4	ug/l	388752	4	13.678	1056150	50.0
unknown13.562	13.562	5.1	ug/l	107872	4	13.678	1056150	50.0
Di-tert-butyl d...	14.651	15.8	ug/l	334513	4	13.678	1056150	50.0
Tetradecane	14.847	7.2	ug/l	152393	4	13.678	1056150	50.0
Tridecane	15.702	7.7	ug/l	162433	4	13.678	1056150	50.0
Trisulfide, bis...	16.327	19.4	ug/l	409229	4	13.678	1056150	50.0