

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
 Data File : VN067455.D
 Acq On : 23 Jun 2021 14:26
 Operator : JC/MD
 Sample : M2802-02
 Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 7 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\82N061421W.M
 Title : SW846 8260

Signal : TIC: VN067455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.217	74	85	103	rVB3	22172	48998	1.16%	0.262%
2	2.410	145	157	168	rBV3	23161	42619	1.01%	0.228%
3	8.018	2227	2248	2256	rBV2	226749	551998	13.04%	2.957%
4	8.077	2260	2270	2289	rVV2	446438	1103435	26.06%	5.910%
5	8.161	2290	2301	2322	rVB3	56932	139938	3.31%	0.750%
6	8.284	2327	2347	2368	rBV2	172142	407462	9.62%	2.182%
7	8.434	2384	2403	2427	rBV	291373	672835	15.89%	3.604%
8	8.552	2427	2447	2464	rVB5	29711	76381	1.80%	0.409%
9	8.820	2531	2547	2568	rVB3	114179	234420	5.54%	1.256%
10	8.965	2580	2601	2633	rBV	658571	1396957	33.00%	7.482%
11	9.456	2758	2784	2797	rBV4	44858	113000	2.67%	0.605%
12	10.443	3133	3152	3163	rBV	1033265	1959362	46.28%	10.494%
13	10.507	3163	3176	3209	rVB	2198909	4233548	100.00%	22.675%
14	11.749	3621	3639	3666	rBV	894249	1649377	38.96%	8.834%
15	11.956	3694	3716	3738	rBV5	70043	140403	3.32%	0.752%
16	12.371	3859	3871	3884	rVV2	29232	52748	1.25%	0.283%
17	12.487	3895	3914	3927	rBV7	25848	66396	1.57%	0.356%
18	12.733	3993	4006	4029	rVB	695587	1247232	29.46%	6.680%
19	12.983	4085	4099	4107	rBV6	37237	69331	1.64%	0.371%
20	13.047	4111	4123	4139	rVB	282617	481693	11.38%	2.580%
21	13.154	4155	4163	4172	rBV2	33449	47073	1.11%	0.252%
22	13.286	4203	4212	4228	rVB2	78765	121550	2.87%	0.651%
23	13.369	4232	4243	4254	rBV2	68063	121019	2.86%	0.648%
24	13.559	4304	4314	4324	rBV9	61929	115820	2.74%	0.620%
25	13.610	4327	4333	4341	rVV7	47633	75822	1.79%	0.406%
26	13.677	4345	4358	4378	rVV	851001	1497188	35.36%	8.019%
27	13.994	4466	4476	4488	rBV	256899	390019	9.21%	2.089%
28	14.477	4639	4656	4660	rBV8	29051	64310	1.52%	0.344%
29	14.651	4704	4721	4740	rVB	232258	444858	10.51%	2.383%
30	14.847	4776	4794	4807	rBV2	134429	234250	5.53%	1.255%
31	14.914	4810	4819	4832	rBV6	48324	91713	2.17%	0.491%
32	15.469	5016	5026	5032	rBV6	29203	52923	1.25%	0.283%
33	15.702	5103	5113	5134	rVB3	117484	212209	5.01%	1.137%
34	16.325	5330	5345	5362	rBV	211976	455156	10.75%	2.438%
35	16.684	5470	5479	5489	rVB3	34741	58365	1.38%	0.313%

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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\82N061421W.M
Title : SW846 8260

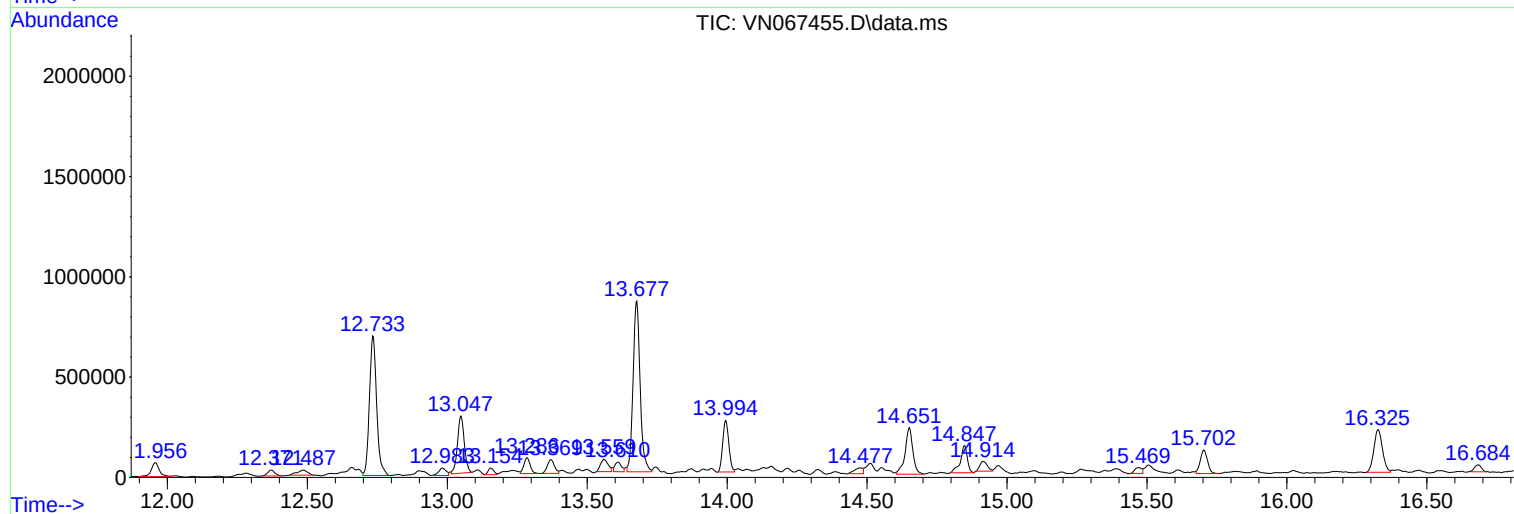
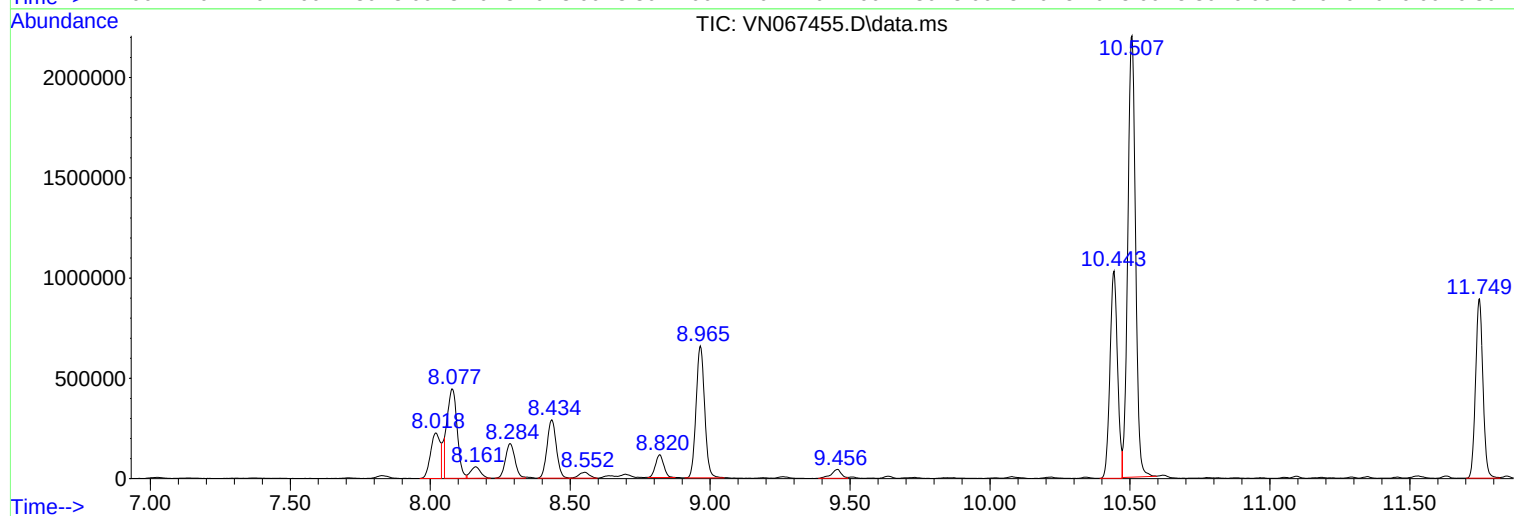
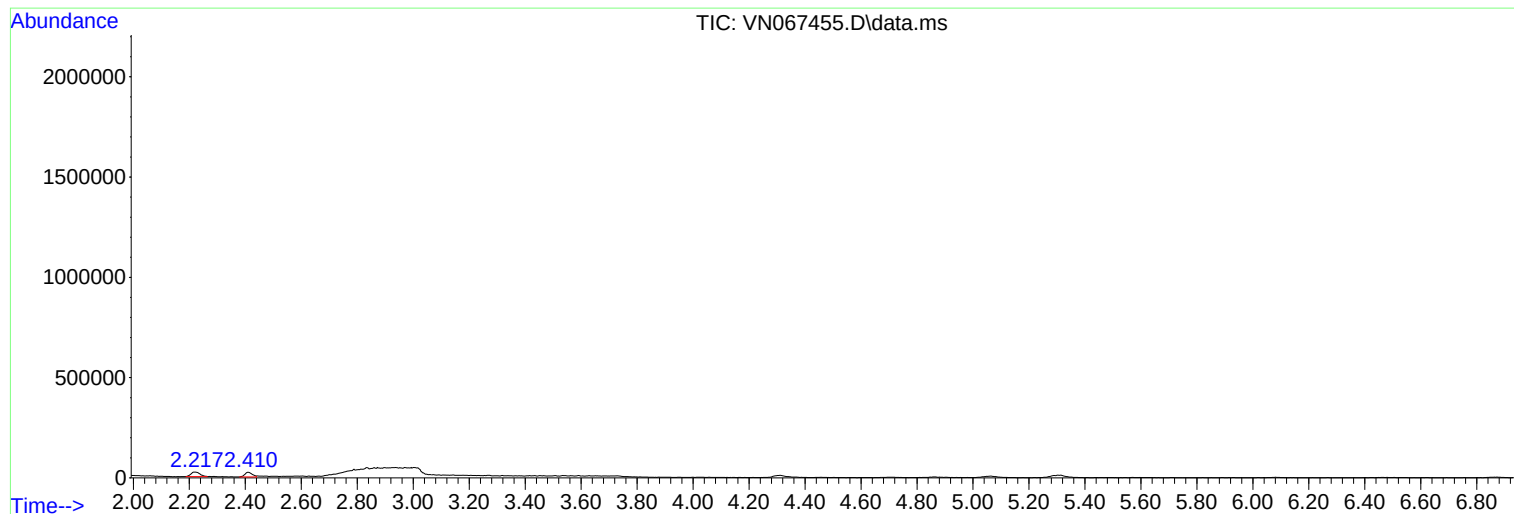
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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



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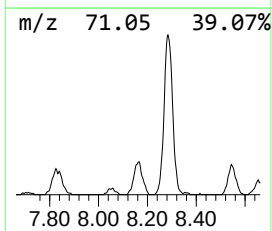
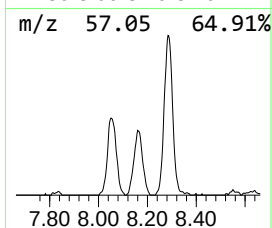
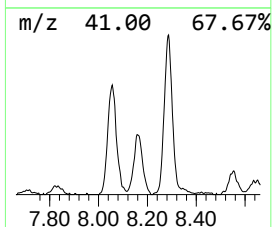
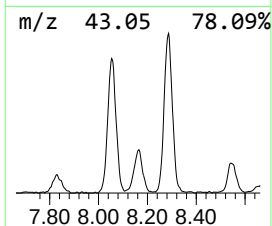
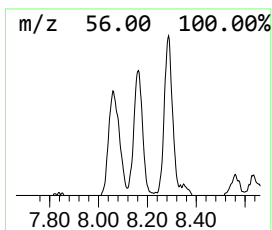
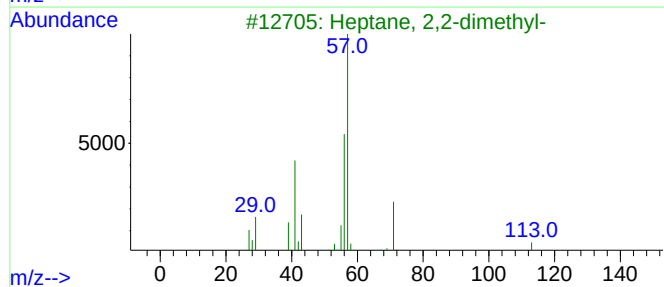
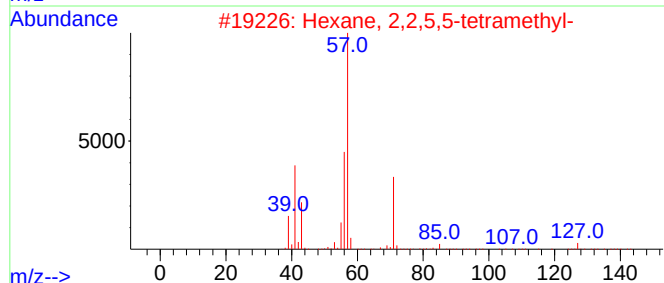
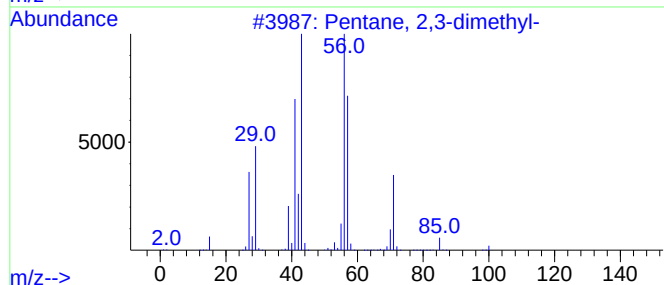
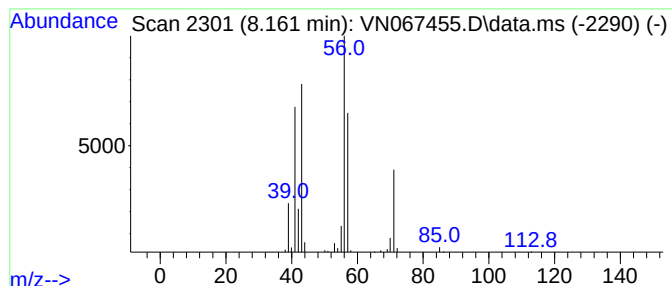
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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	6.34 ug/l	139938	Pentafluorobenzene	8.083

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	74
2			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	64
3			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	50
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	46
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	43



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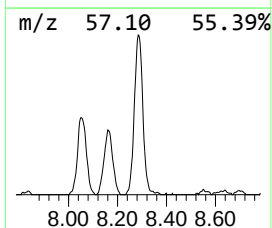
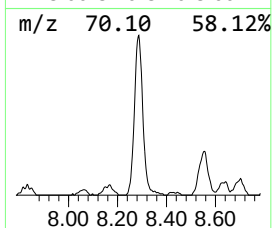
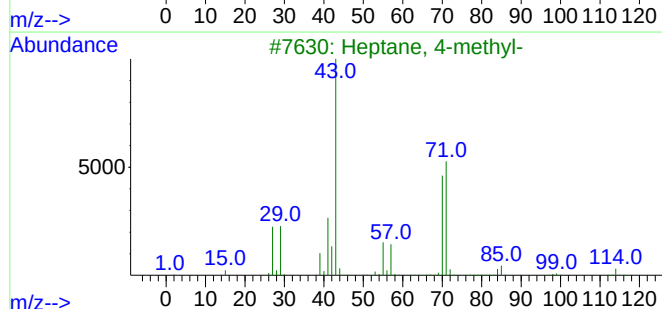
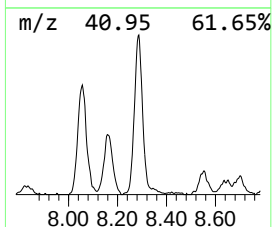
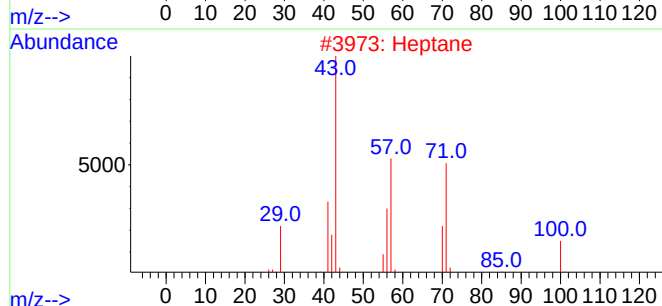
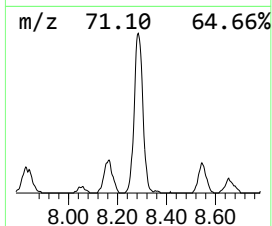
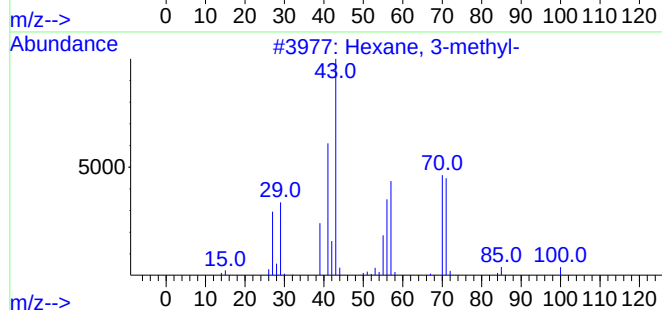
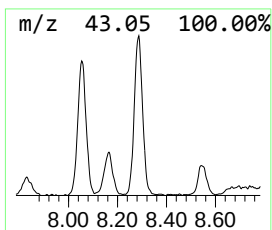
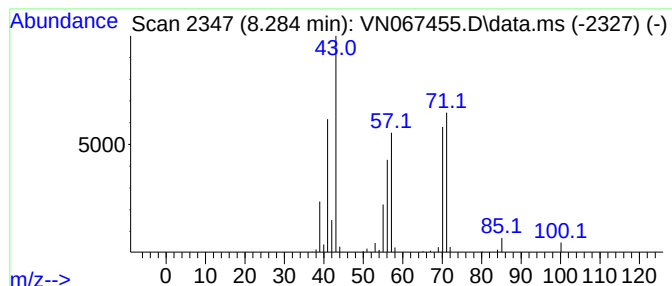
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.284	18.46 ug/l	407462	Pentafluorobenzene	8.083

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	80
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	50



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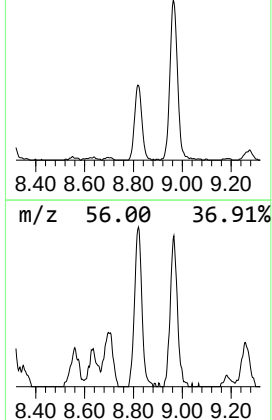
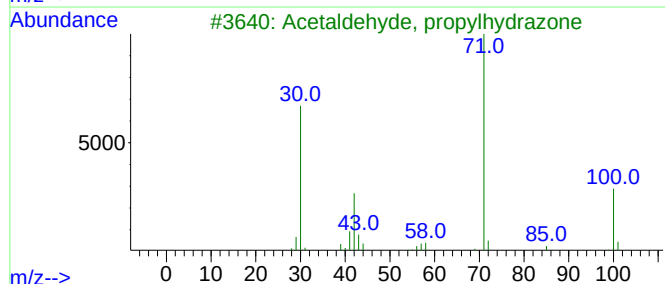
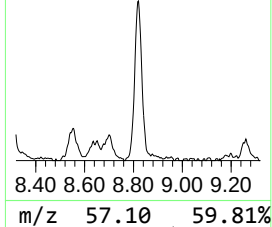
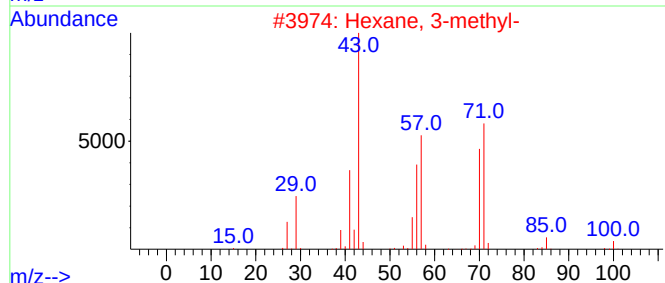
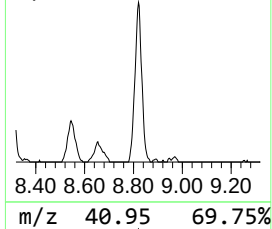
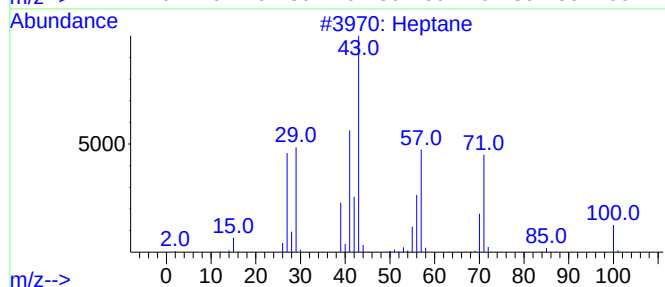
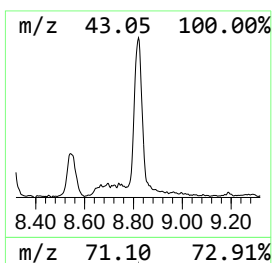
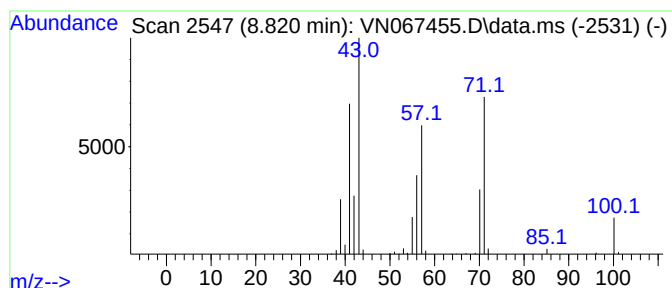
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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.
8.820	8.39 ug/l	234420	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane	100	C7H16	000142-82-5	86
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	40
3			Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38
4			Cyclobutanone, 3-ethyl-	98	C6H10O	056335-73-0	35
5			3-Hexanone	100	C6H12O	000589-38-8	27



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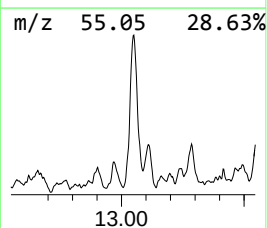
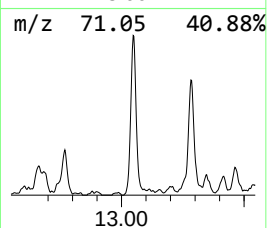
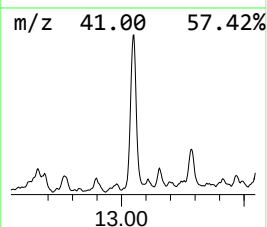
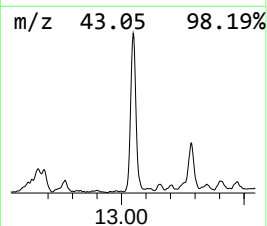
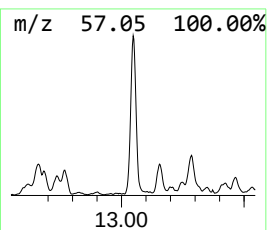
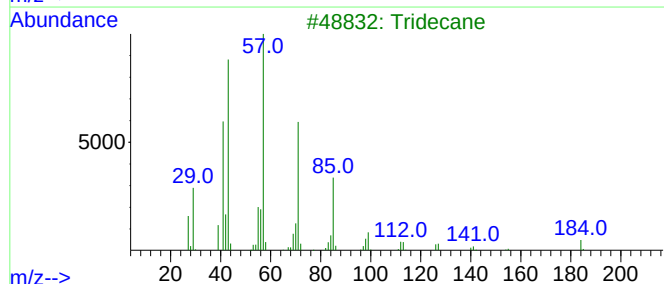
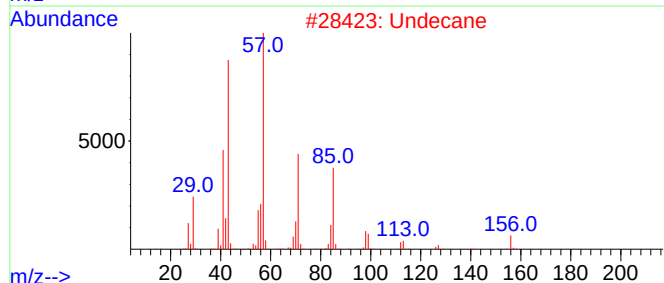
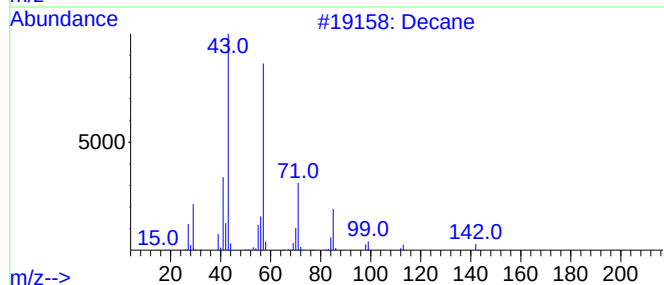
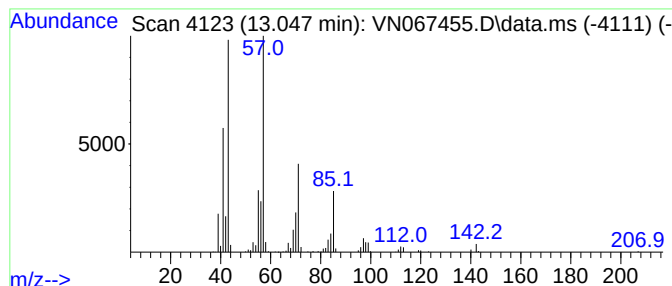
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.047	16.09 ug/l	481693	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	91
2			Undecane	156	C11H24	001120-21-4	78
3			Tridecane	184	C13H28	000629-50-5	72
4			Oxalic acid, allyl decyl ester	270	C15H26O4	1000309-23-8	72
5			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	64



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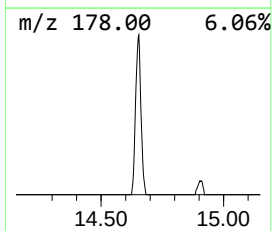
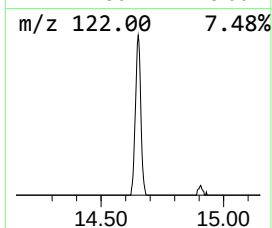
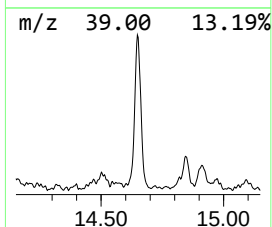
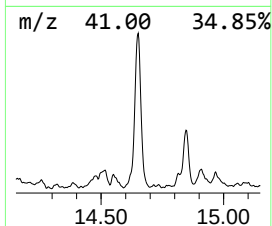
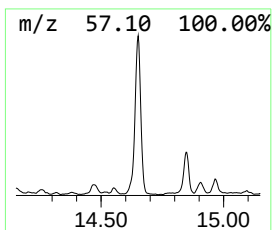
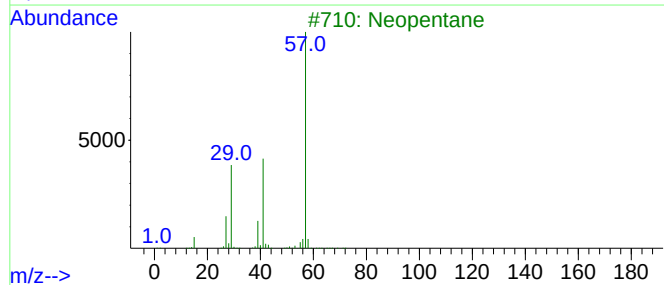
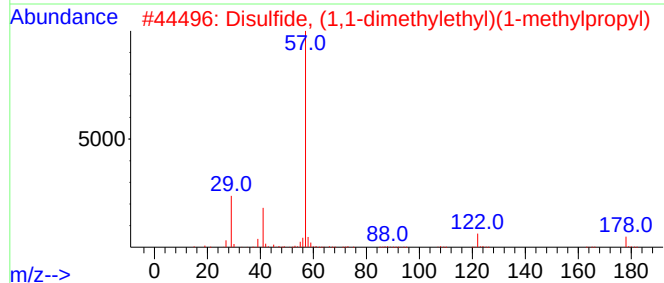
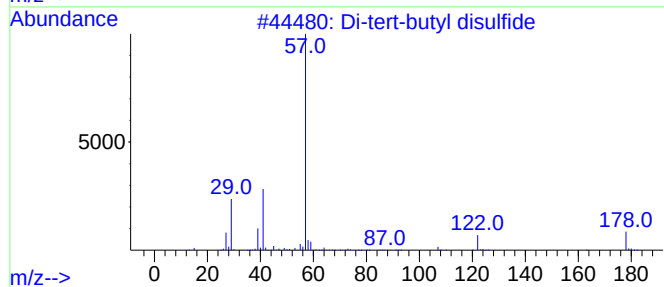
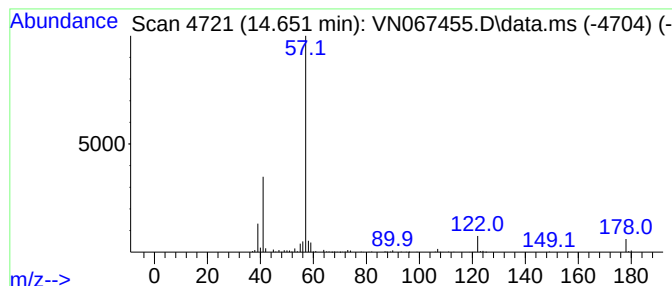
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Quant Title : SW846 8260

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

Peak Number 5 Di-tert-butyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.651	14.86 ug/l	444858	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	90
2			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	87
3			Neopentane	72	C5H12	000463-82-1	47
4			Disulfide, dibutyl	178	C8H18S2	000629-45-8	43
5			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067455.D
Acq On : 23 Jun 2021 14:26
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

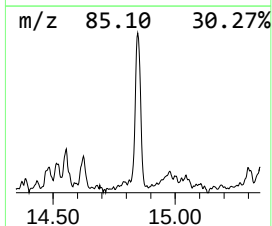
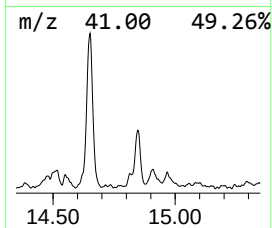
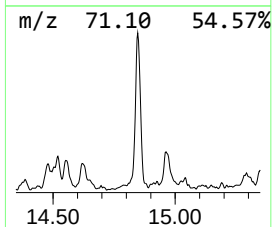
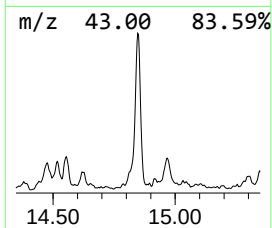
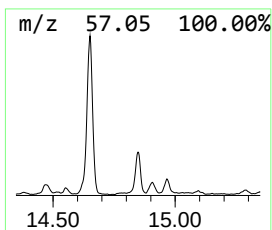
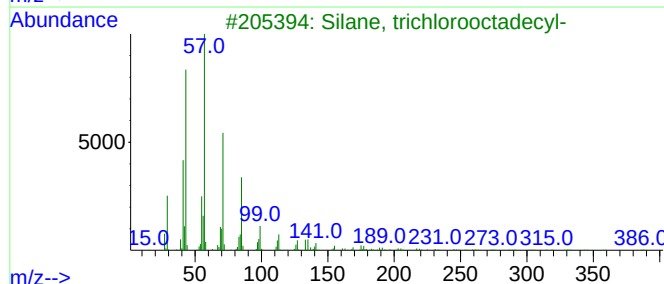
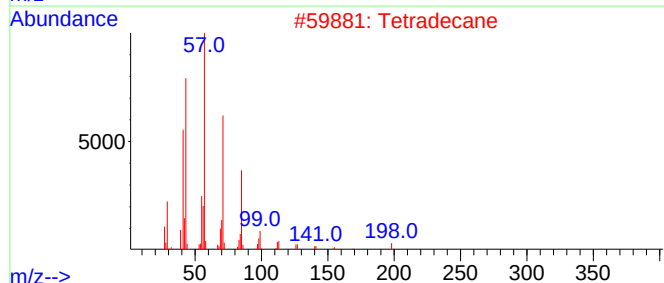
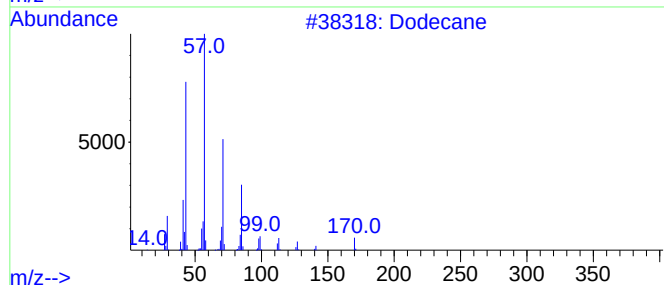
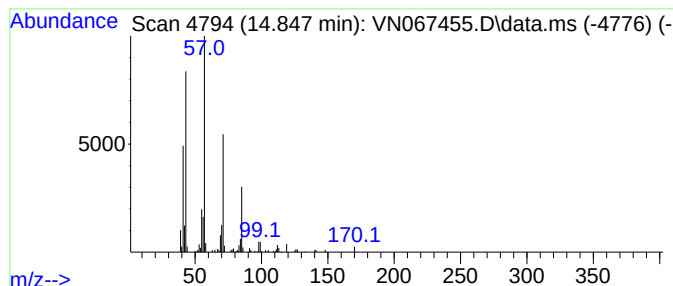
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Quant Title : SW846 8260

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

Peak Number 6 Dodecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.847	7.82 ug/l	234250	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Tetradecane	198	C14H30	000629-59-4	86
3			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	78
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067455.D
Acq On : 23 Jun 2021 14:26
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

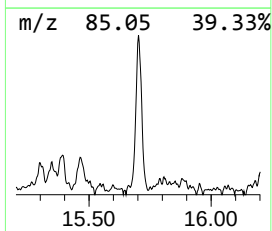
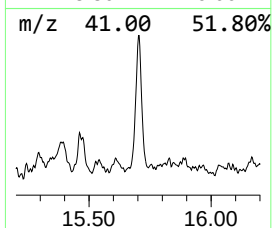
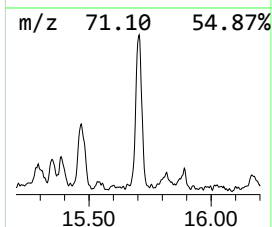
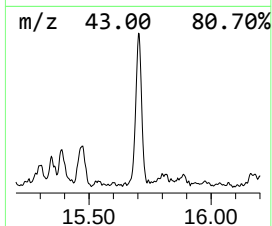
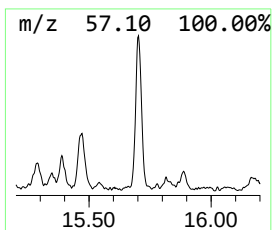
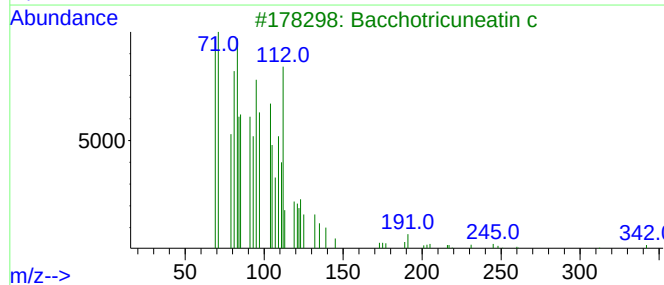
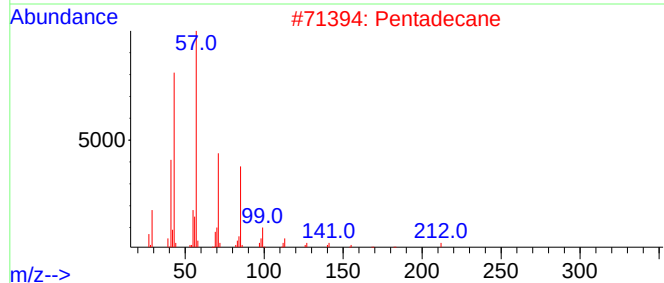
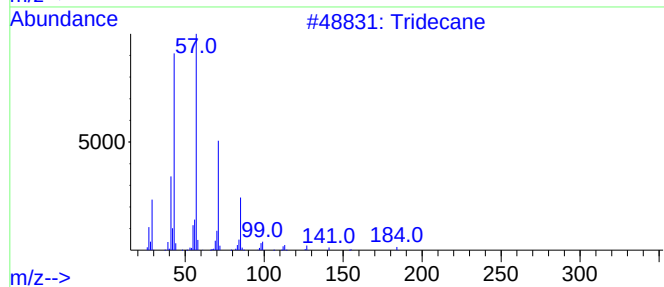
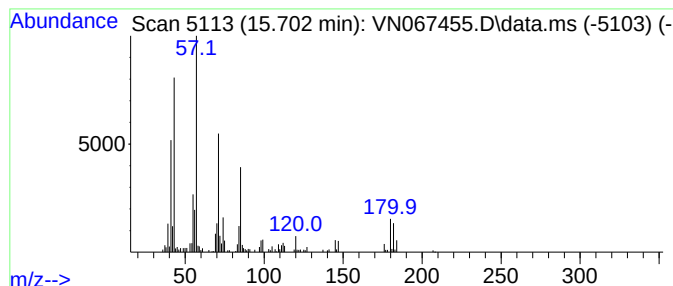
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Quant Title : SW846 8260

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

Peak Number 7 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.702	7.09 ug/l	212209	1,4-Dichlorobenzene-d4	13.677

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	81
2		Pentadecane	212	C15H32	000629-62-9	59
3		Bacchotricuneatin c	342	C20H22O5	066563-30-2	58
4		Tetradecane	198	C14H30	000629-59-4	58
5		Hexadecane	226	C16H34	000544-76-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067455.D
Acq On : 23 Jun 2021 14:26
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

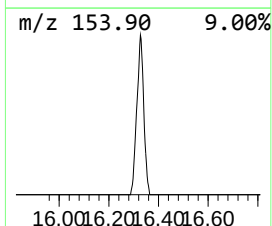
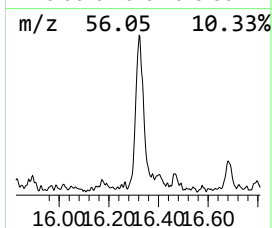
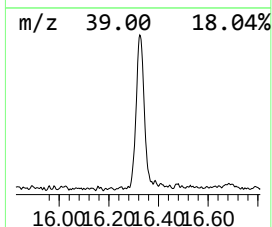
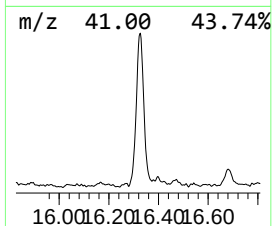
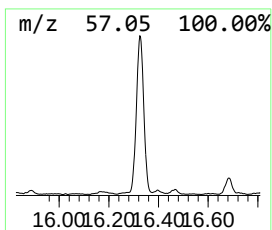
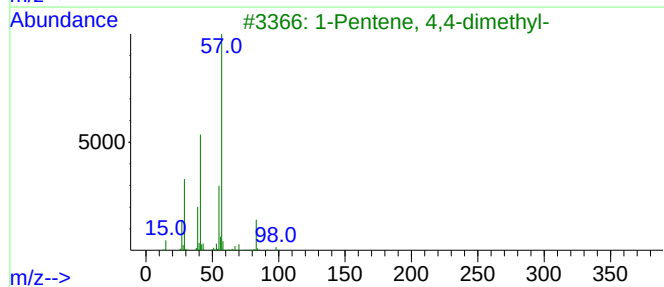
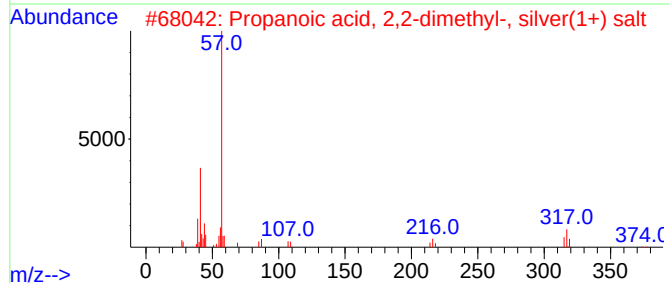
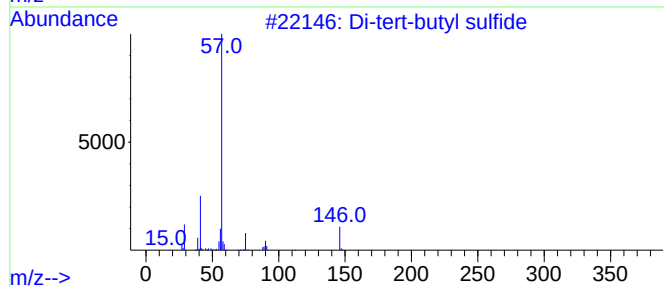
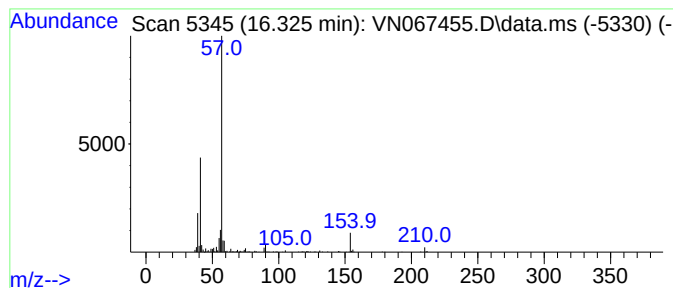
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown16.325 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.325	15.20 ug/l	455156	1,4-Dichlorobenzene-d4	13.677

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl sulfide	146	C8H18S	000107-47-1	59
2			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	38
3			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	32
4			Butane, 2-bromo-	136	C4H9Br	000078-76-2	32
5			Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062321\
Data File : VN067455.D
Acq On : 23 Jun 2021 14:26
Operator : JC/MD
Sample : M2802-02
Misc : 1.10g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41817

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.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	6.3	ug/l	139938	1	8.083	1103440	50.0
Hexane, 3-methyl-	8.284	18.5	ug/l	407462	1	8.083	1103440	50.0
Heptane	8.820	8.4	ug/l	234420	2	8.965	1396960	50.0
Decane	13.047	16.1	ug/l	481693	4	13.677	1497190	50.0
Di-tert-butyl d...	14.651	14.9	ug/l	444858	4	13.677	1497190	50.0
Dodecane	14.847	7.8	ug/l	234250	4	13.677	1497190	50.0
Tridecane	15.702	7.1	ug/l	212209	4	13.677	1497190	50.0
unknown16.325	16.325	15.2	ug/l	455156	4	13.677	1497190	50.0