LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

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\82N120221W.M
Title : SW846 8260

Signal : TIC: VN070174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.529	189	201	217	rVB2	217925	396377	3.36%	0.524%
2	3.840	675	690	724	rVB3	58120	197048	1.67%	0.261%
3	3.985	724	744	767	rBV4	54769	148925	1.26%	0.197%
4	5.385	1238	1266	1303	rBV3	356357	1279145	10.85%	1.692%
5	5.621	1327	1354	1388	rVB3	330454	1165772	9.89%	1.542%
6	6.498	1650	1681	1704	rVB6	83940	323939	2.75%	0.428%
7	6.897	1806	1830	1847	rBV5	39956	134468	1.14%	0.178%
8	7.844	2168	2183	2204	rVB	290077	733012	6.22%	0.970%
9	8.024	2226	2250	2260	rBV2	615699	1455281	12.34%	1.925%
10	8.088	2261	2274	2294	rVV2	1143708	2689566	22.81%	3.557%
11	8.440	2383	2405	2423	rBV	792451	1907185	16.18%	2.523%
12	8.539	2423	2442	2463	rBV	5174087	11790205	100.00%	15.595%
13	8.968	2583	2602	2635	rBV	1913350	4254074	36.08%	5.627%
14	9.427	2757	2773	2784	rBV4	60471	141029	1.20%	0.187%
15	9.732	2868	2887	2904	rBV4	62801	139512	1.18%	0.185%
16	9.882	2930	2943	2957	rVB4	126811	245354	2.08%	0.325%
17	9.974	2958	2977	2988	rBV	858377	1714974	14.55%	2.268%
18	10.207	3045	3064	3066	rBV2	1299410	2079407	17.64%	2.750%
19	10.237	3068	3075	3102	rVB	2530757	4706511	39.92%	6.225%
20	10.443	3135	3152	3167	rBV	2625531	4892533	41.50%	6.471%
21	10.553	3180	3193	3214	rVB	2580060	4730384	40.12%	6.257%
22	10.859	3294	3307	3328	rVV2	273797	553136	4.69%	0.732%
23	11.089	3379	3393	3420	rBV2	259190	536006	4.55%	0.709%
24	11.213	3420	3439	3469	rVV3	517063	1251920	10.62%	1.656%
25	11.618	3575	3590	3619	rBV3	485480	1214411	10.30%	1.606%
26	11.744	3620	3637	3663	rVV	3424188	6552174	55.57%	8.666%
27	11.856	3665	3679	3699	rVV5	607009	1433354	12.16%	1.896%
28	11.956	3701	3716	3739	rVV	786415	1655830	14.04%	2.190%
29	12.041	3740	3748	3760	rVB3	80251	124979	1.06%	0.165%
30	12.280	3822	3837	3849	rBV3	204930	398422	3.38%	0.527%
31	12.358	3855	3866	3876	rBV2	119052	203648	1.73%	0.269%
32	12.538	3920	3933	3945	rBV7	141105	325831	2.76%	0.431%
33	12.731	3989	4005	4031	rVB2	1758039	3224068	27.35%	4.264%
34	12.846	4036	4048	4059	rBV3	164999	333438	2.83%	0.441%
35	12.986	4089	4100	4105	rBV2	230123	368304	3.12%	0.487%
36	13.061	4121	4128	4147	rVB2	246463	439884	3.73%	0.582%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
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Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

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\82N120221W.M
Title : SW846 8260

37	13.222	4176	4188	4199	rBV	161325	285869	2.42%	0.378%
38	13.369	4232	4243	4259	rVB	811213	1397445	11.85%	1.848%
39	13.675	4342	4357	4386	rBV2	1916464	4085412	34.65%	5.404%
40	13.876	4424	4432	4440	rBV2	153470	254231	2.16%	0.336%
41	13.919	4441	4448	4469	rVB2	261157	449333	3.81%	0.594%
42	14.217	4549	4559	4571	rVB	91008	146154	1.24%	0.193%
43	14.815	4770	4782	4796	rBV7	109417	224884	1.91%	0.297%
44	14.933	4809	4826	4840	rBV2	119364	272080	2.31%	0.360%
45	15.083	4870	4882	4897	rBV5	64318	122902	1.04%	0.163%
46	15.507	5022	5040	5061	rVB	1508033	2972712	25.21%	3.932%
47	15.611	5068	5079	5094	rVB4	93194	178813	1.52%	0.237%
48	16.620	5438	5455	5479	rVB	640534	1474460	12.51%	1.950%

Sum of corrected areas: 75604401

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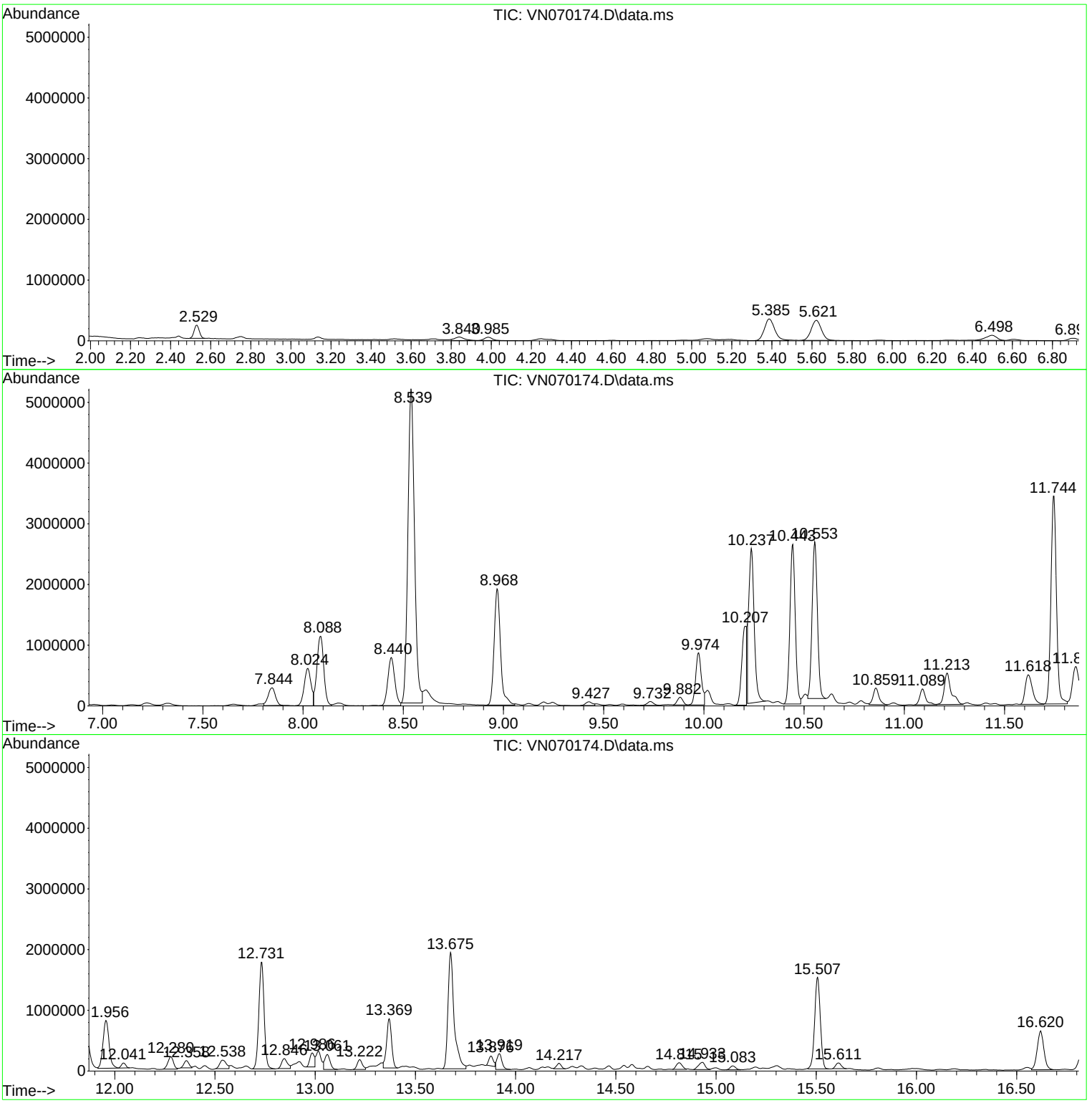
Instrument :
MSVOA_N
ClientSampleId :
MW-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

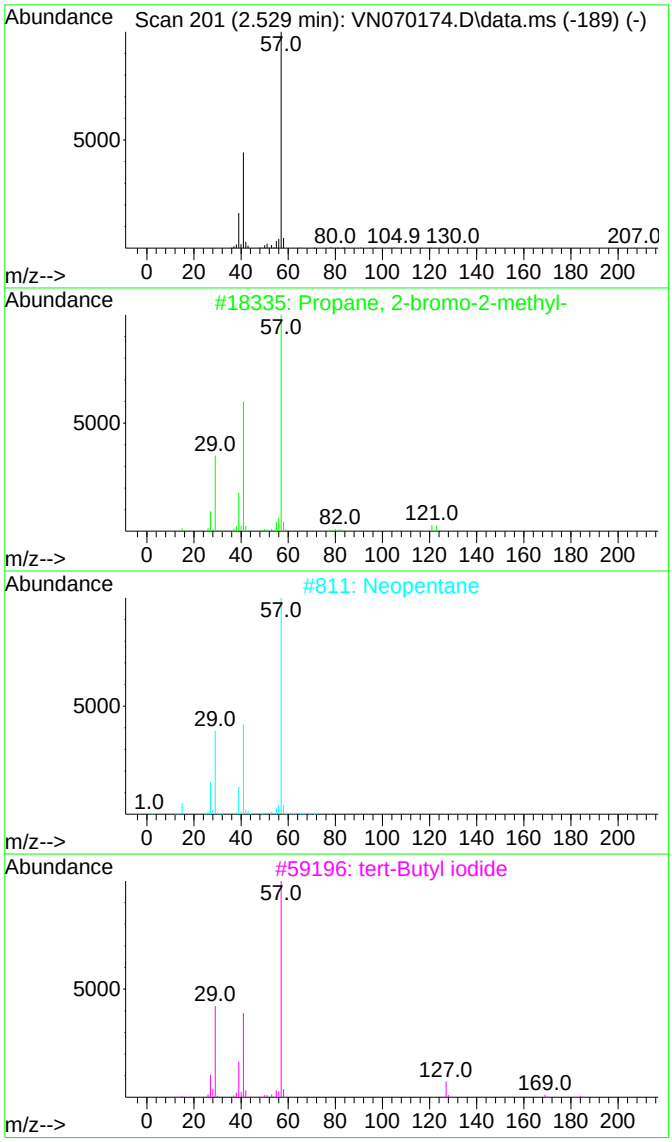
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

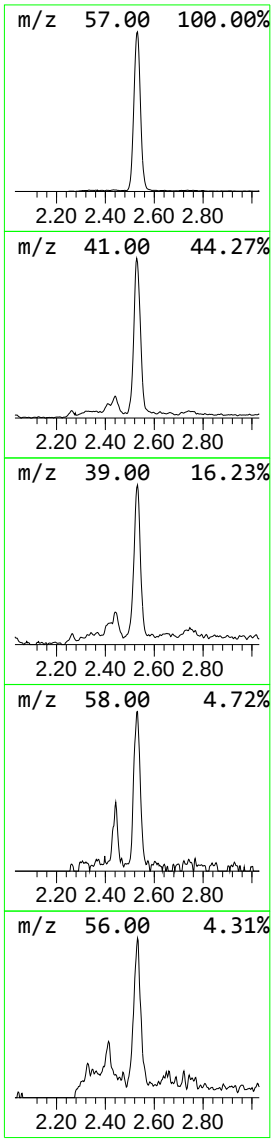
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane, 2-bromo-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.529	7.37 ug/l	396377	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	72
2	Neopentane	72	C5H12	000463-82-1	64
3	tert-Butyl iodide	184	C4H9I	000558-17-8	50
4	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	45
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

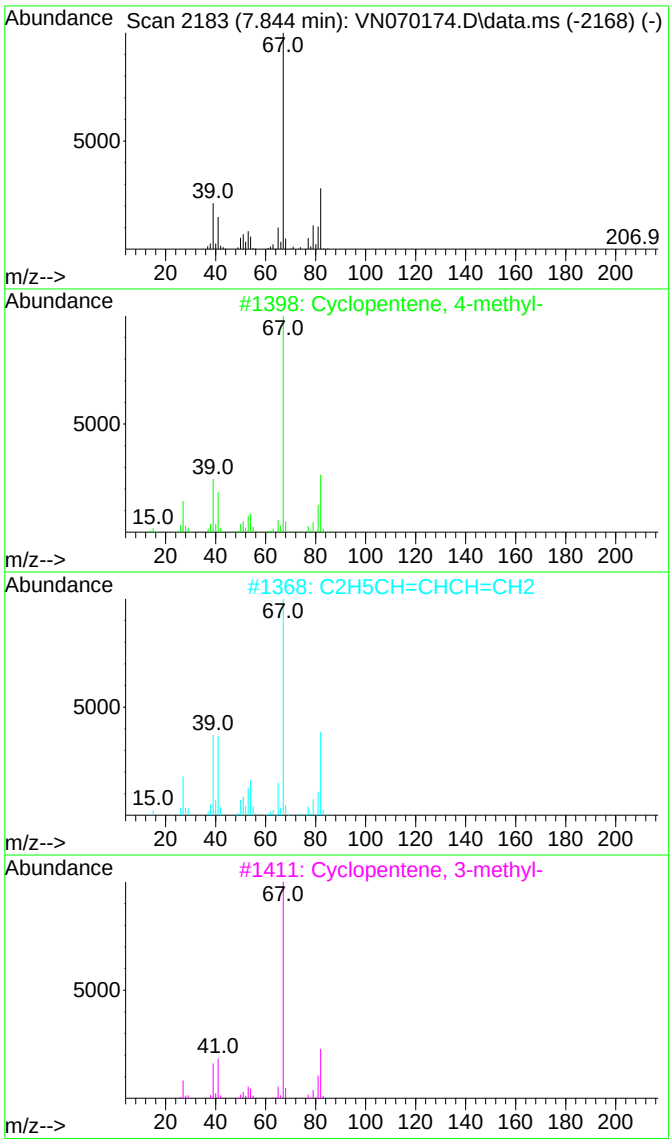
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

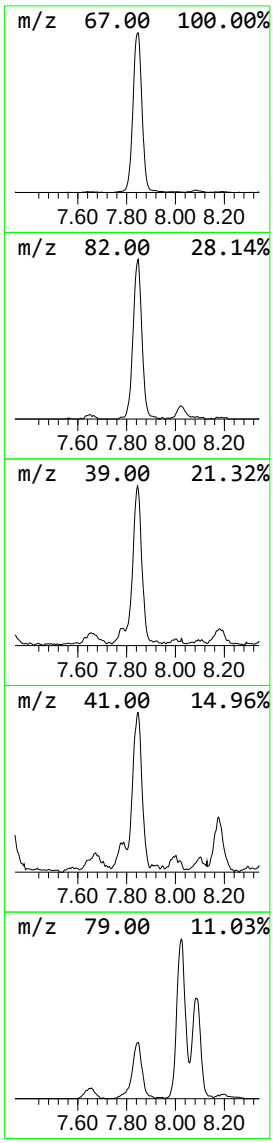
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Cyclopentene, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.844	13.63 ug/l	733012	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	87
2	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	83
3	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	80
4	2,4-Hexadiene, (E,Z)-	82	C6H10	005194-50-3	80
5	1,4-Hexadiene	82	C6H10	000592-45-0	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

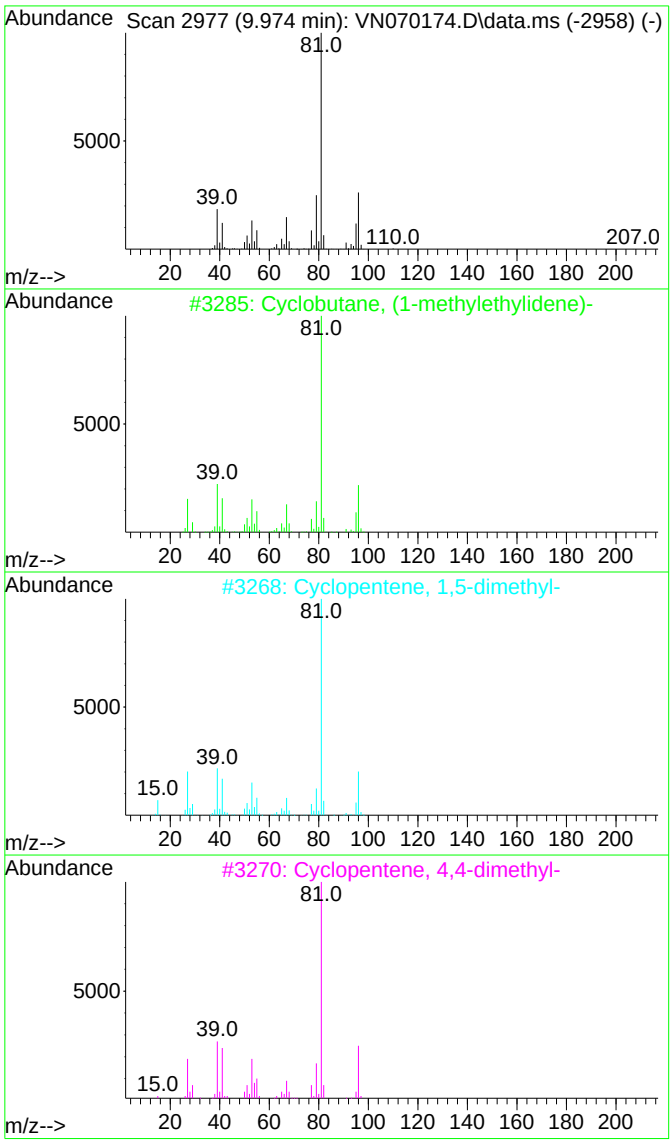
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

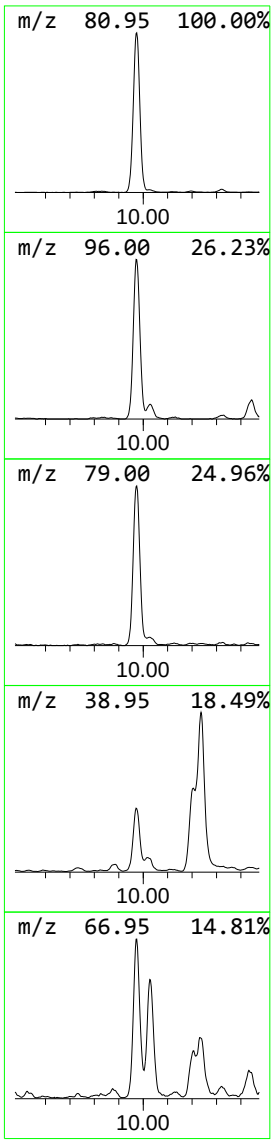
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclobutane, (1-methylethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.974	20.16 ug/l	1714970	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
2	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	90
3	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	86
4	3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	78
5	1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	72





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Data File : VN070174.D
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Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

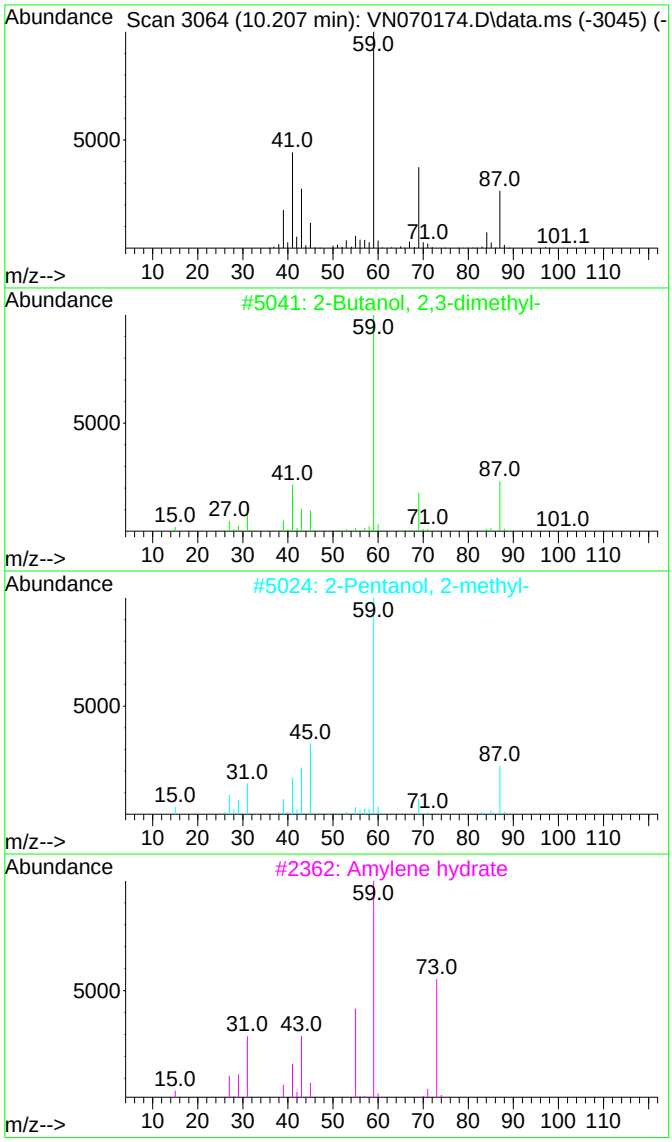
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

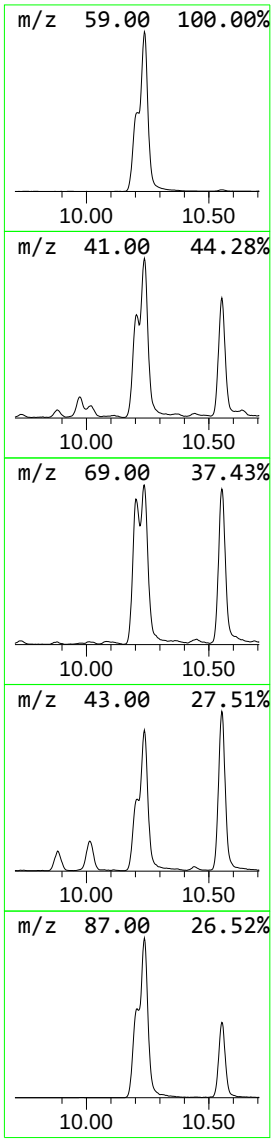
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butanol, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.207	24.44 ug/l	2079410	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	83
3	Amylene hydrate	88	C5H12O	000075-85-4	45
4	2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	45
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45





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Instrument :
MSVOA_N
ClientSampleId :
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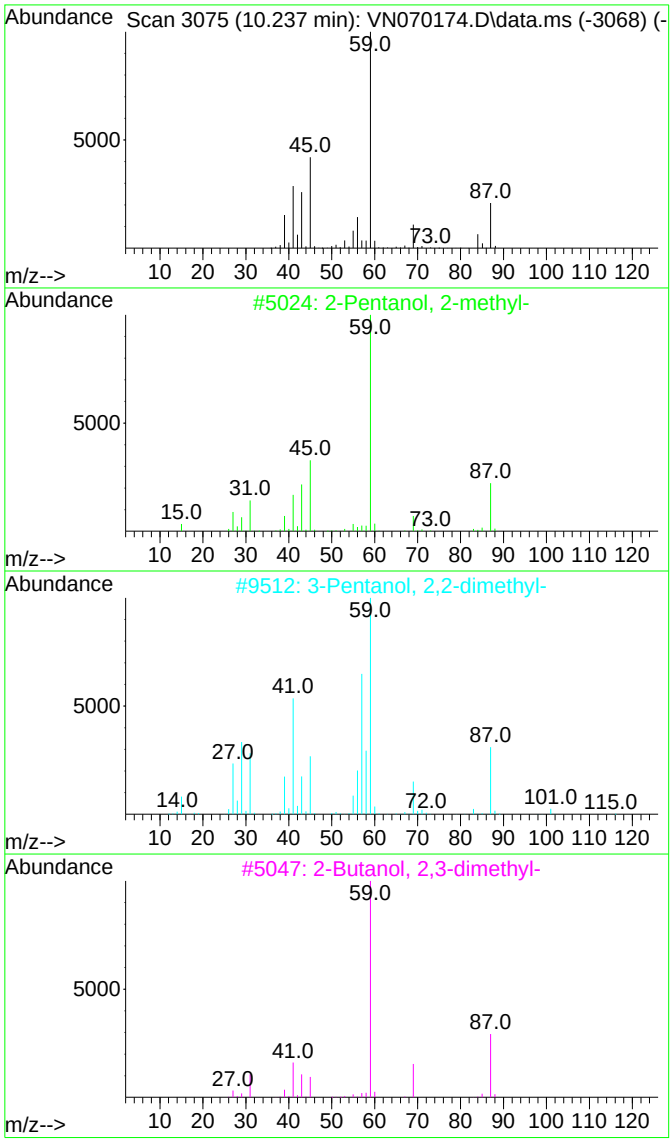
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

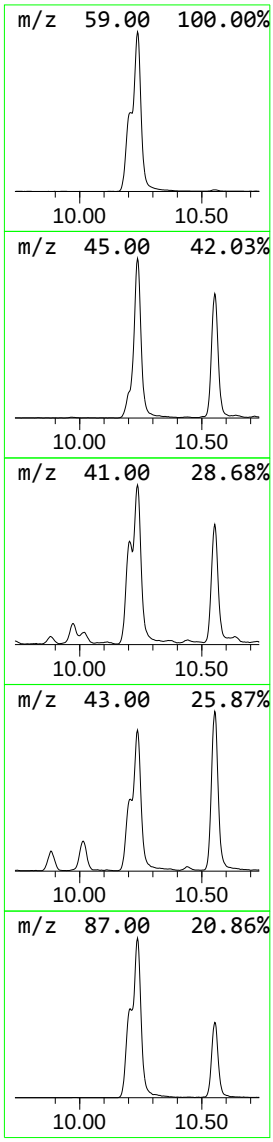
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Pentanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.236	55.32 ug/l	4706510	1,4-Difluorobenzene	8.968

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
2	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	45
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	42
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	40
5	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	38





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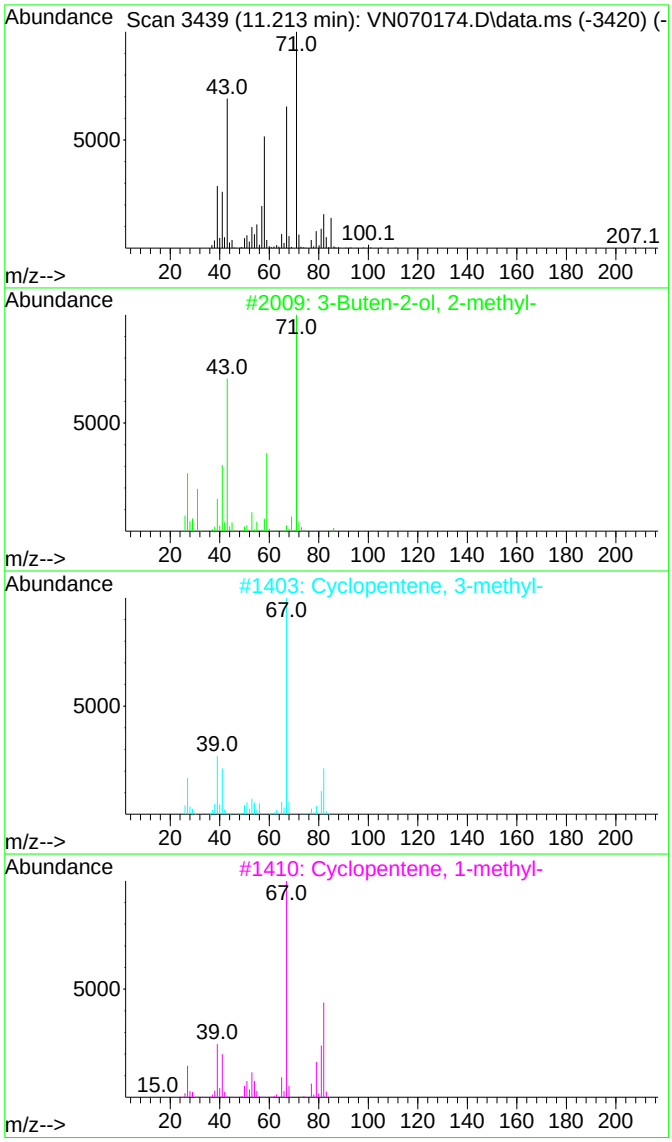
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

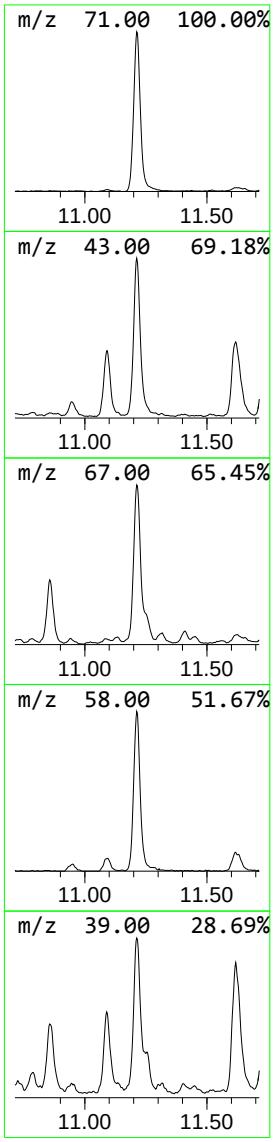
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown11.213 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.213	9.55 ug/l	1251920	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	38
2	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	25
3	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	25
4	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	25
5	1,4-Pentadiene, 3-methyl-	82	C6H10	001115-08-8	15





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ClientSampleId :
MW-30

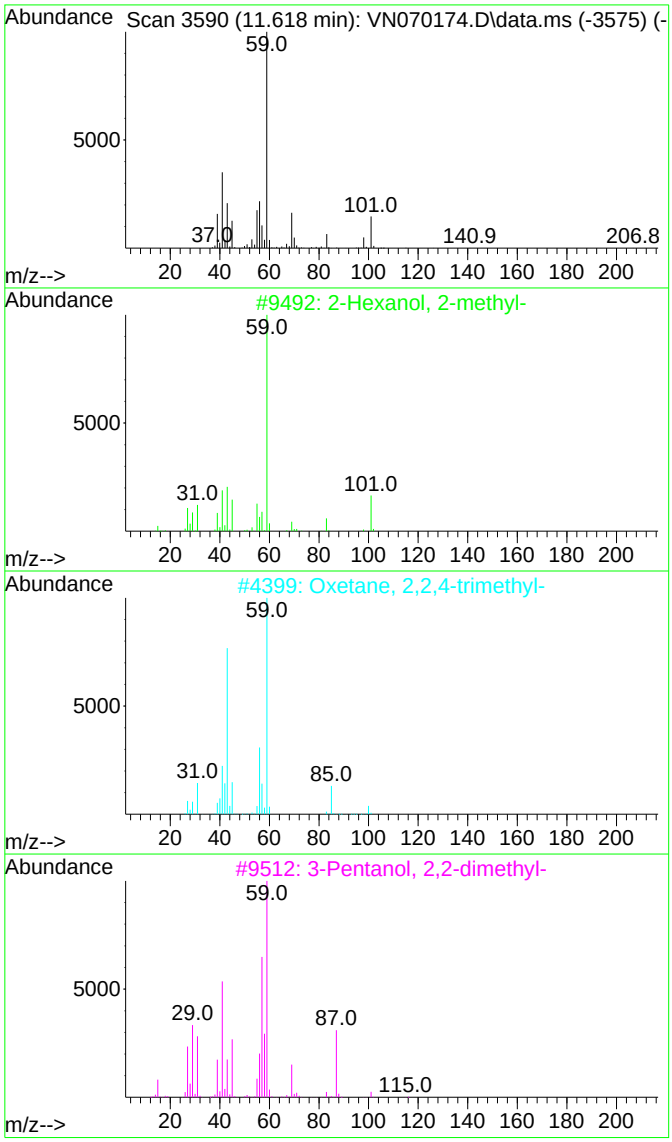
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

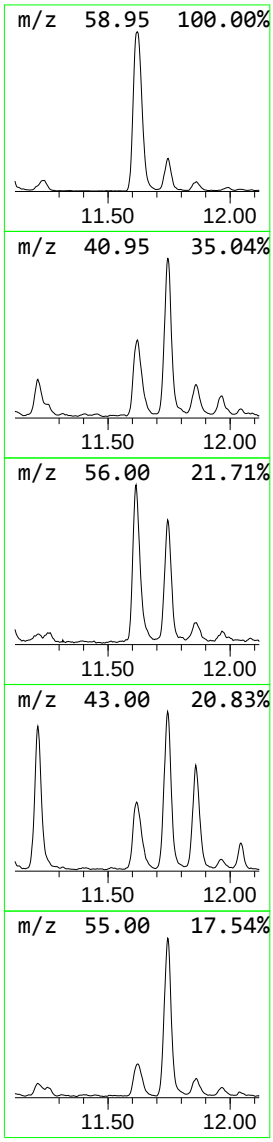
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Hexanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.618	9.27 ug/l	1214410	Chlorobenzene-d5	11.746

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	72
2	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	59
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	53
4	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	50
5	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	47





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Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

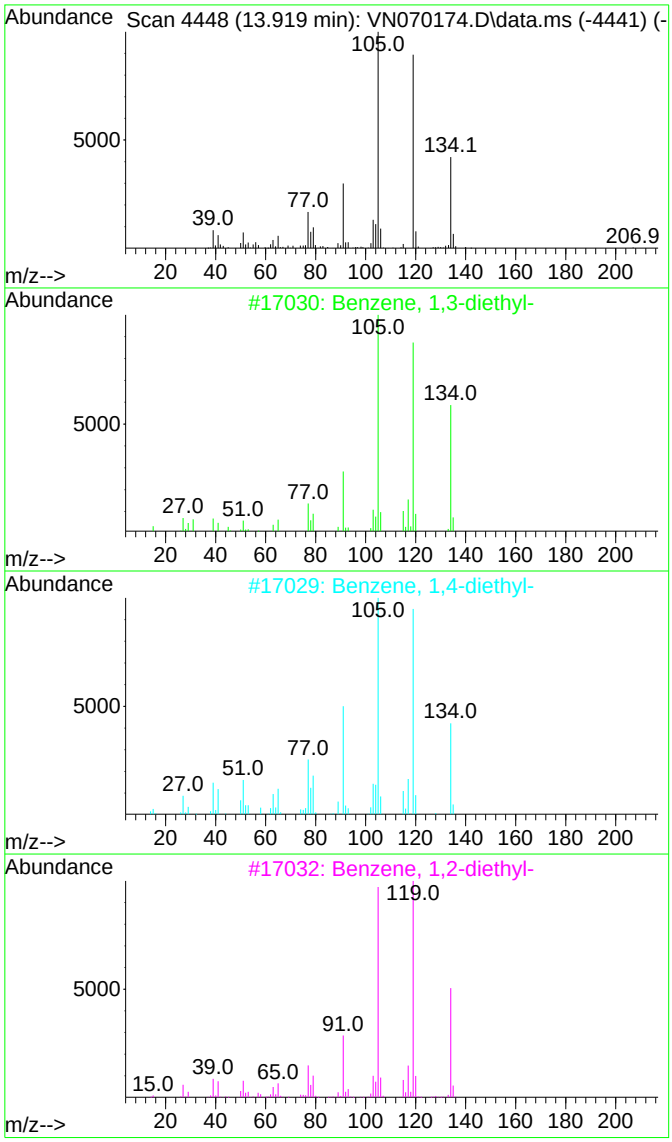
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

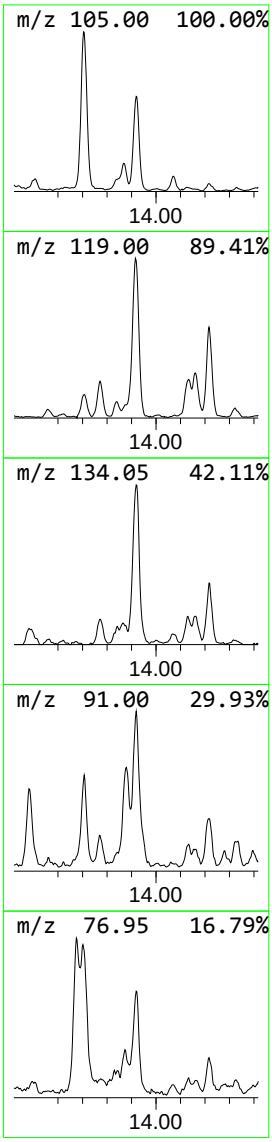
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,3-diethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.919	5.50 ug/l	449333	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	91
2	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	91
3	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	91
4	Benzene, tert-butyl-	134	C10H14	000098-06-6	68
5	Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	64





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Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

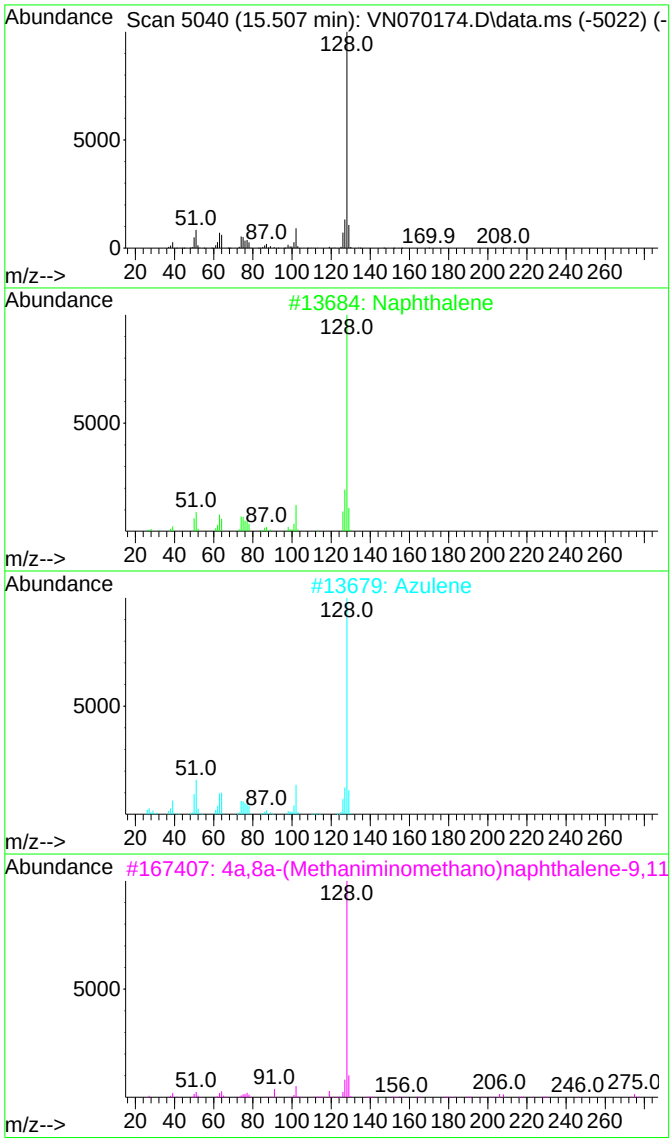
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

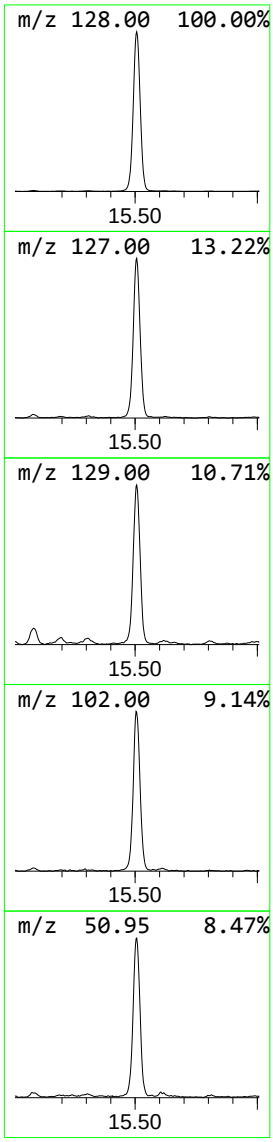
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.507	36.38 ug/l	2972710	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	97
2	Azulene	128	C10H8	000275-51-4	94
3	4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	74
4	4-Phenylbut-3-ene-1-yne	128	C10H8	1000222-12-0	64
5	1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

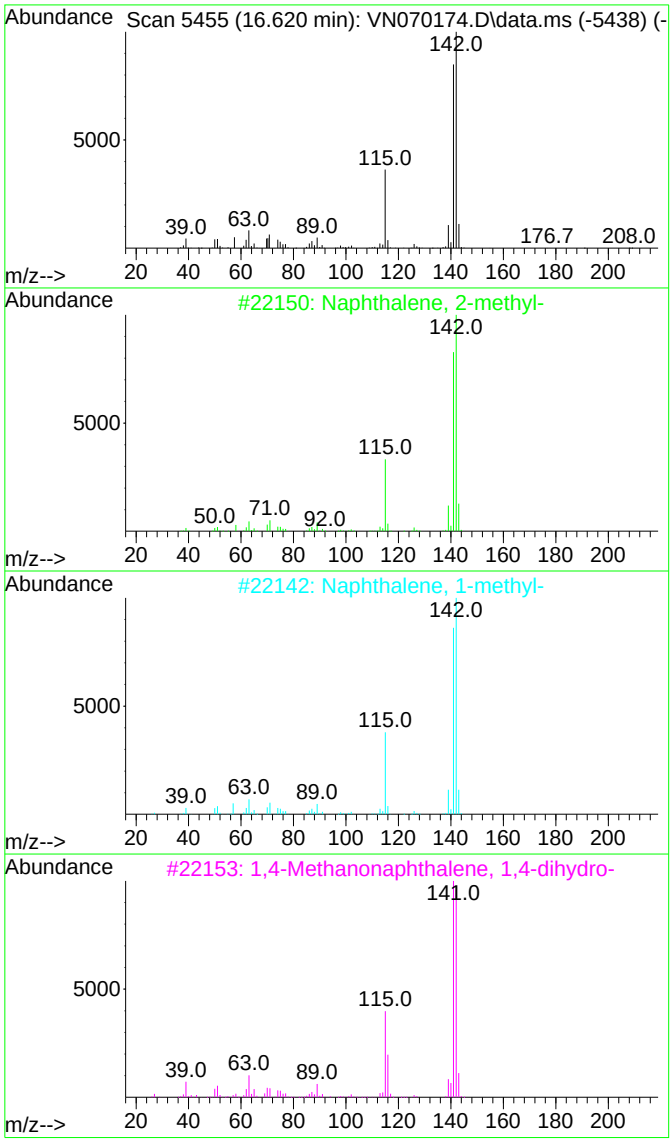
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

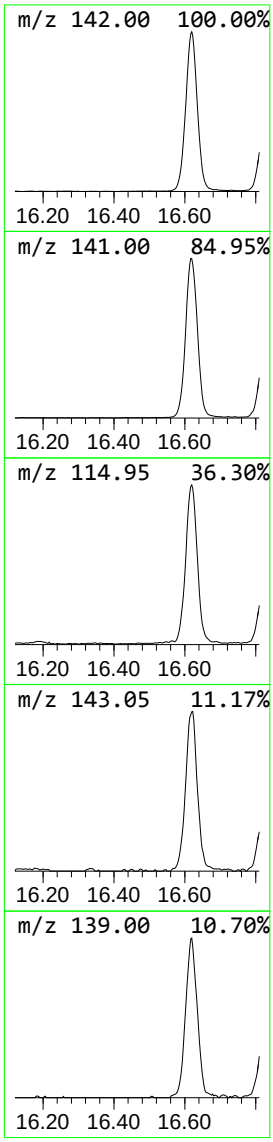
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.620	18.05 ug/l	1474460	1,4-Dichlorobenzene-d4	13.675

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121721\
Data File : VN070174.D
Acq On : 17 Dec 2021 19:35
Operator : JC/MD
Sample : M5039-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-30

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2-brom...	2.529	7.4	ug/l	396377	1	8.086	2689570	50.0
Cyclopentene, 4...	7.844	13.6	ug/l	733012	1	8.086	2689570	50.0
Cyclobutane, (1...	9.974	20.2	ug/l	1714970	2	8.968	4254070	50.0
2-Butanol, 2,3-...	10.207	24.4	ug/l	2079410	2	8.968	4254070	50.0
2-Pentanol, 2-m...	10.236	55.3	ug/l	4706510	2	8.968	4254070	50.0
unknown11.213	11.213	9.6	ug/l	1251920	3	11.746	6552170	50.0
2-Hexanol, 2-me...	11.618	9.3	ug/l	1214410	3	11.746	6552170	50.0
Benzene, 1,3-di...	13.919	5.5	ug/l	449333	4	13.675	4085410	50.0
Azulene	15.507	36.4	ug/l	2972710	4	13.675	4085410	50.0
1,4-Methanonaph...	16.620	18.1	ug/l	1474460	4	13.675	4085410	50.0