LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

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\82N051022W.M
Title : SW846 8260

Signal : TIC: VN072455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	37	43	54	rBV4	10671	30359	2.97%	0.418%
2	2.440	72	77	83	rVB2	9309	15083	1.48%	0.208%
3	2.769	125	133	137	rVB5	8346	17871	1.75%	0.246%
4	3.122	181	193	208	rBV	122540	293449	28.70%	4.039%
5	4.257	373	386	400	rBV4	13795	53844	5.27%	0.741%
6	5.081	512	526	548	rBV3	43181	218551	21.37%	3.008%
7	5.616	604	617	632	rBV2	78845	270339	26.44%	3.721%
8	7.039	849	859	869	rBV5	12337	39090	3.82%	0.538%
9	7.145	869	877	887	rVB4	11208	31224	3.05%	0.430%
10	7.833	983	994	1002	rBV7	8191	25646	2.51%	0.353%
11	8.022	1016	1026	1031	rBV	145103	354139	34.63%	4.874%
12	8.086	1031	1037	1045	rVV	256798	589701	57.67%	8.116%
13	8.175	1045	1052	1062	rVB2	43137	107991	10.56%	1.486%
14	8.433	1088	1096	1109	rBV	180685	422618	41.33%	5.816%
15	8.569	1109	1119	1122	rBV4	25190	63620	6.22%	0.876%
16	8.622	1123	1128	1129	rBV2	14241	20392	1.99%	0.281%
17	8.710	1138	1143	1151	rVB6	8453	19674	1.92%	0.271%
18	8.963	1177	1186	1200	rBV	353689	739809	72.35%	10.182%
19	9.422	1256	1264	1267	rBV3	8136	16505	1.61%	0.227%
20	9.880	1336	1342	1349	rVB3	15203	30091	2.94%	0.414%
21	10.016	1359	1365	1372	rVB2	24142	52361	5.12%	0.721%
22	10.198	1389	1396	1402	rBV6	8171	20137	1.97%	0.277%
23	10.439	1428	1437	1450	rBV	552644	1022567	100.00%	14.073%
24	10.545	1450	1455	1460	rBV6	7072	14376	1.41%	0.198%
25	10.857	1502	1508	1515	rVB4	10921	24089	2.36%	0.332%
26	11.739	1650	1658	1670	rBV	450689	829015	81.07%	11.410%
27	12.574	1792	1800	1808	rBV2	58118	94156	9.21%	1.296%
28	12.727	1819	1826	1837	rBV	343032	590405	57.74%	8.126%
29	13.215	1904	1909	1914	rVB2	8109	12245	1.20%	0.169%
30	13.492	1948	1956	1964	rVB2	10481	23578	2.31%	0.325%
31	13.668	1979	1986	1999	rBV	351687	600760	58.75%	8.268%
32	13.833	2008	2014	2017	rBV2	22846	37484	3.67%	0.516%
33	13.874	2017	2021	2026	rVV	43819	70393	6.88%	0.969%
34	13.933	2026	2031	2036	rVB5	7058	14109	1.38%	0.194%
35	13.998	2036	2042	2047	rBV3	9554	13570	1.33%	0.187%
36	14.127	2058	2064	2070	rBV2	8795	13636	1.33%	0.188%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

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\82N051022W.M
Title : SW846 8260

37	14.209	2073	2078	2084	rBV2	26461	40387	3.95%	0.556%
38	14.321	2091	2097	2104	rVB	88723	144371	14.12%	1.987%
39	14.533	2128	2133	2138	rBV2	8836	13888	1.36%	0.191%
40	14.804	2175	2179	2184	rBV2	15932	23807	2.33%	0.328%
41	14.927	2192	2200	2206	rBV4	74612	142661	13.95%	1.963%
42	15.080	2220	2226	2229	rBV3	5925	10862	1.06%	0.149%
43	15.192	2239	2245	2248	rBV5	8865	15429	1.51%	0.212%
44	15.304	2257	2264	2276	rVB3	13415	33211	3.25%	0.457%
45	15.498	2289	2297	2305	rBV2	22435	48433	4.74%	0.667%

Sum of corrected areas: 7265926

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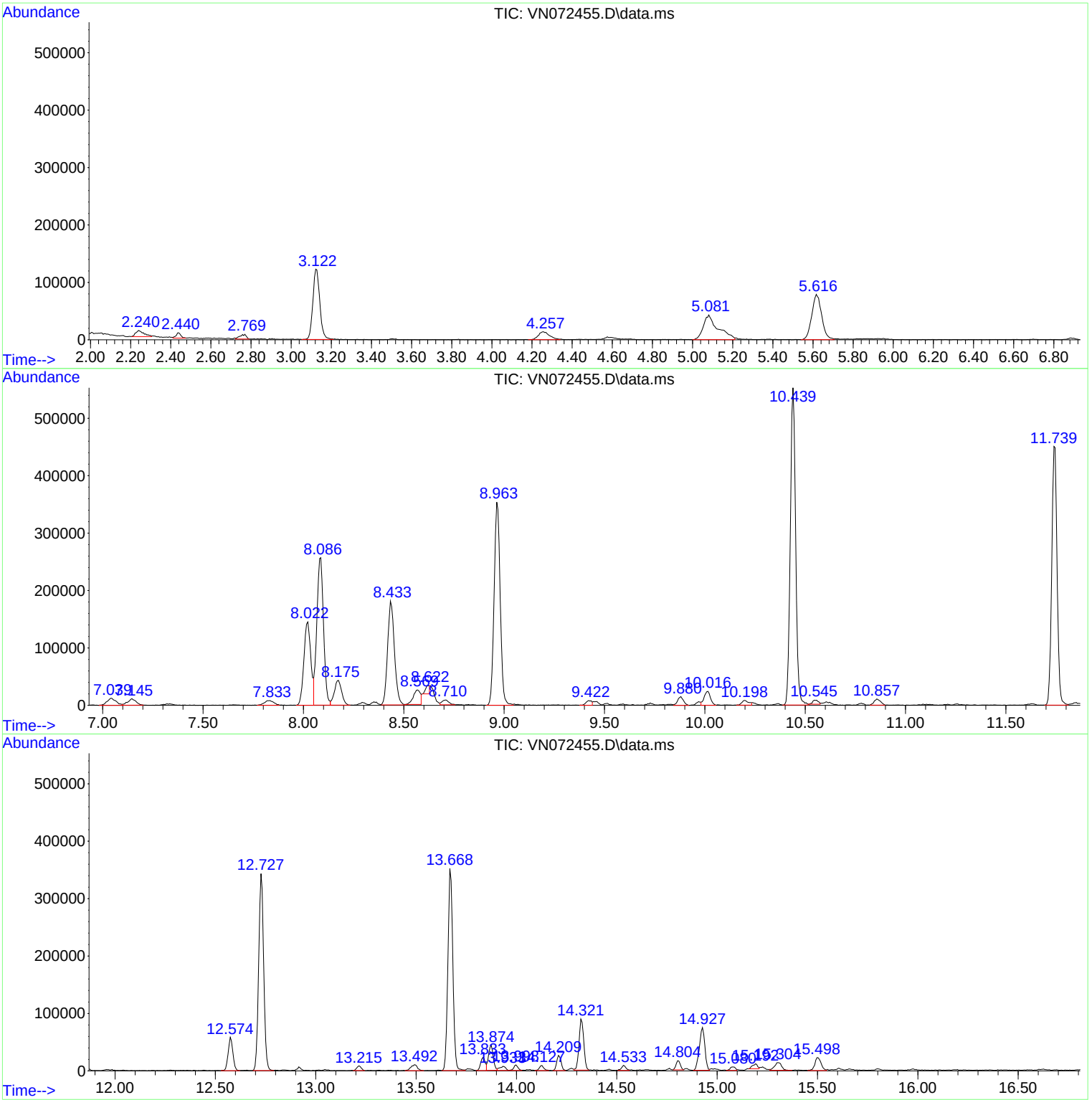
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

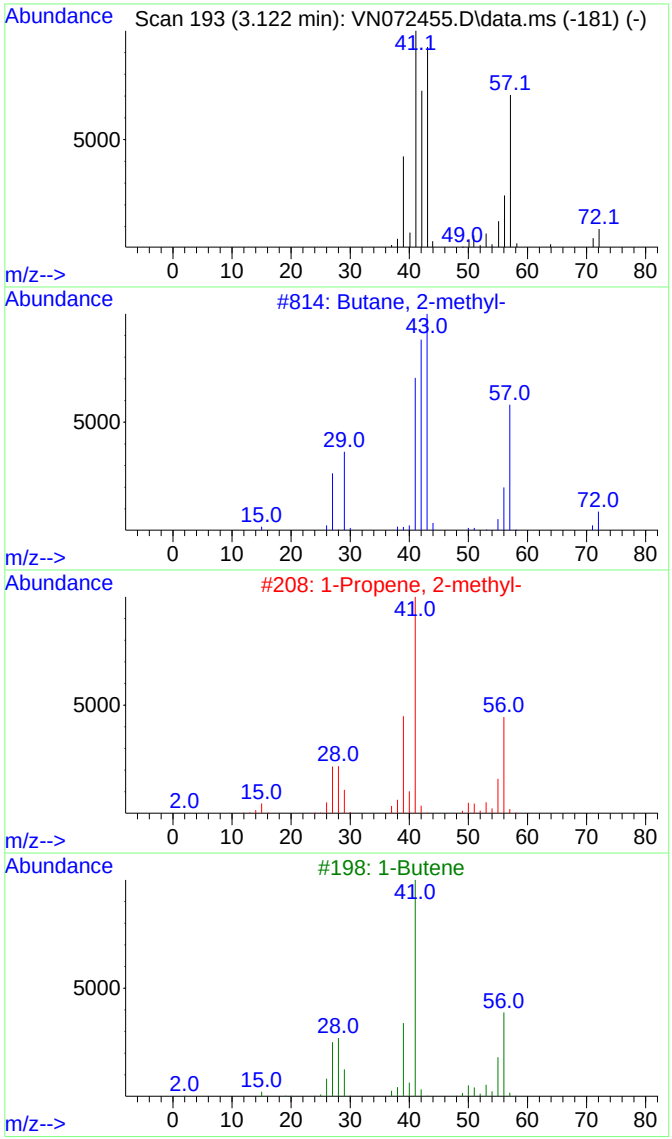
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

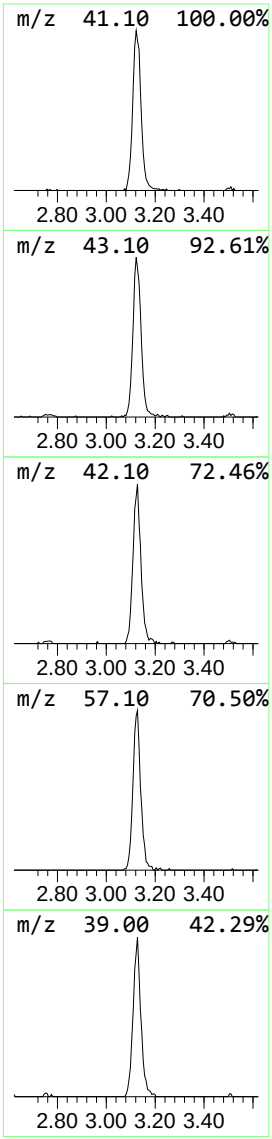
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.122	24.88 ug/l	293449	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	50
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	38
3	1-Butene	56	C4H8	000106-98-9	38
4	3-Buten-1-ol	72	C4H8O	000627-27-0	28
5	Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

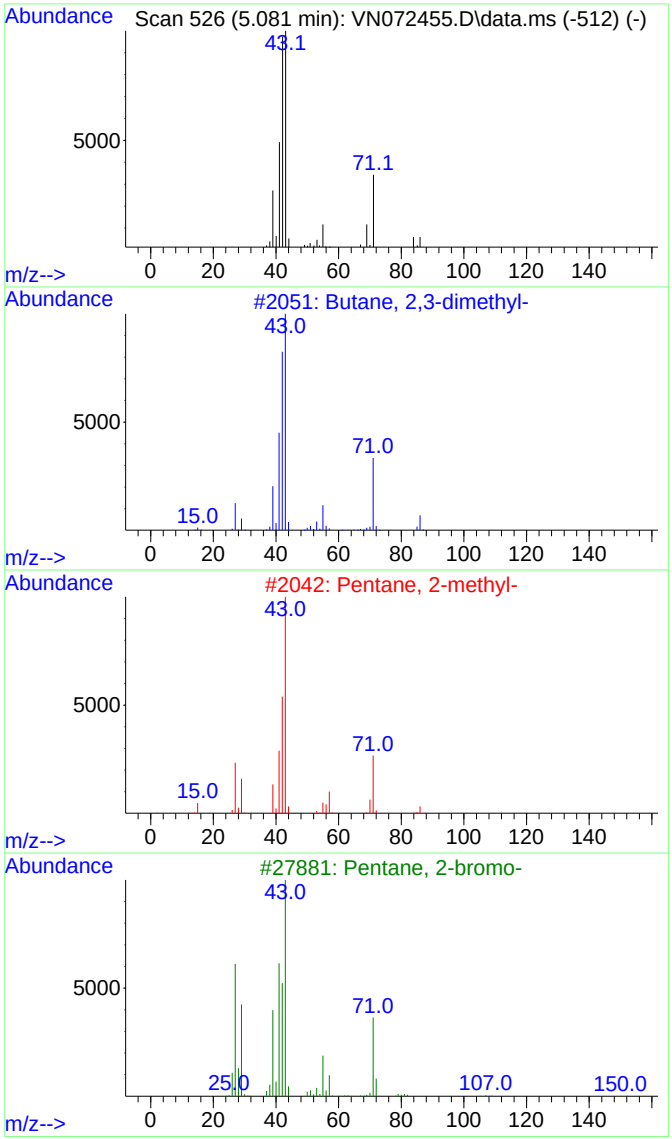
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

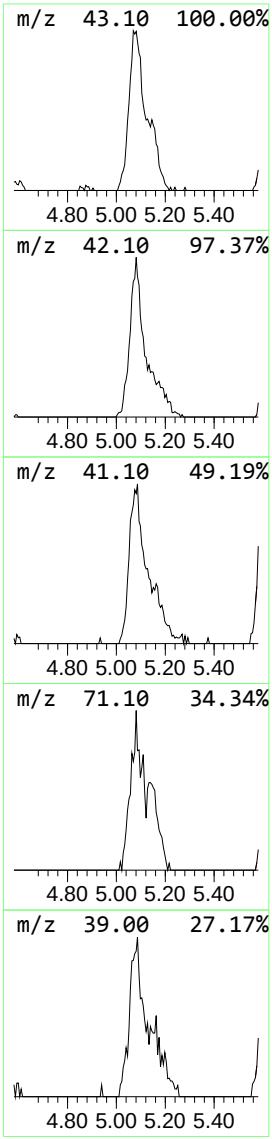
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	18.53 ug/l	218551	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	53
3	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	43
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	43
5	1-Pentene	70	C5H10	000109-67-1	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

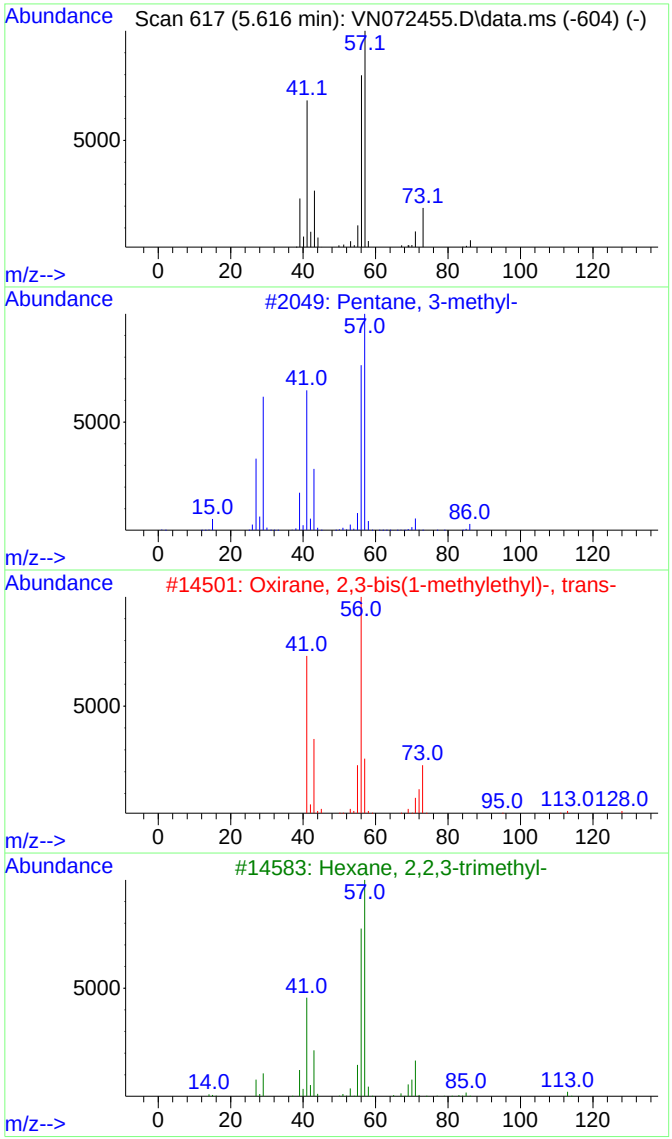
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

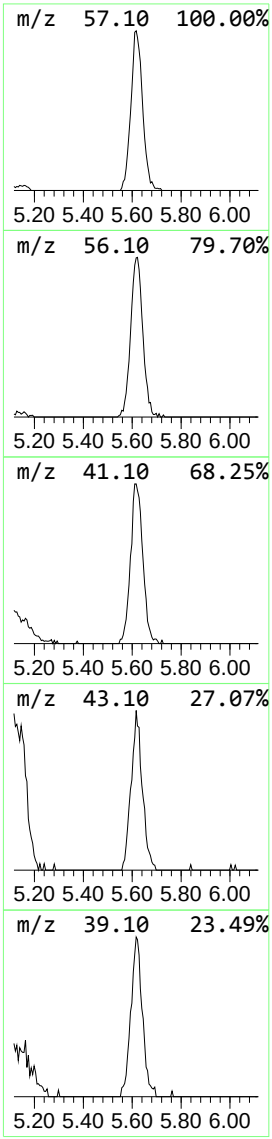
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.616	22.92 ug/l	270339	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	74
2	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	64
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
5	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

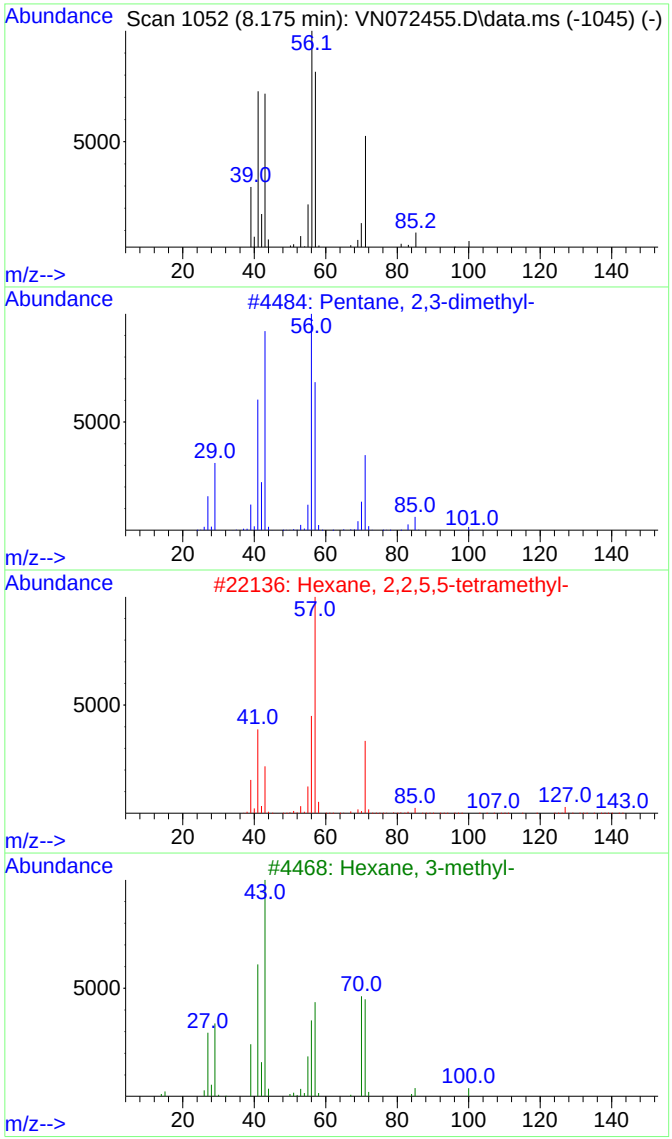
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

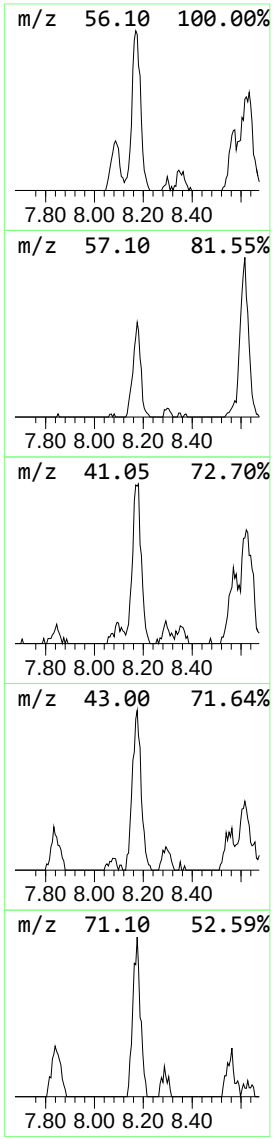
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	9.16 ug/l	107991	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	59
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	47
4	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	43
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

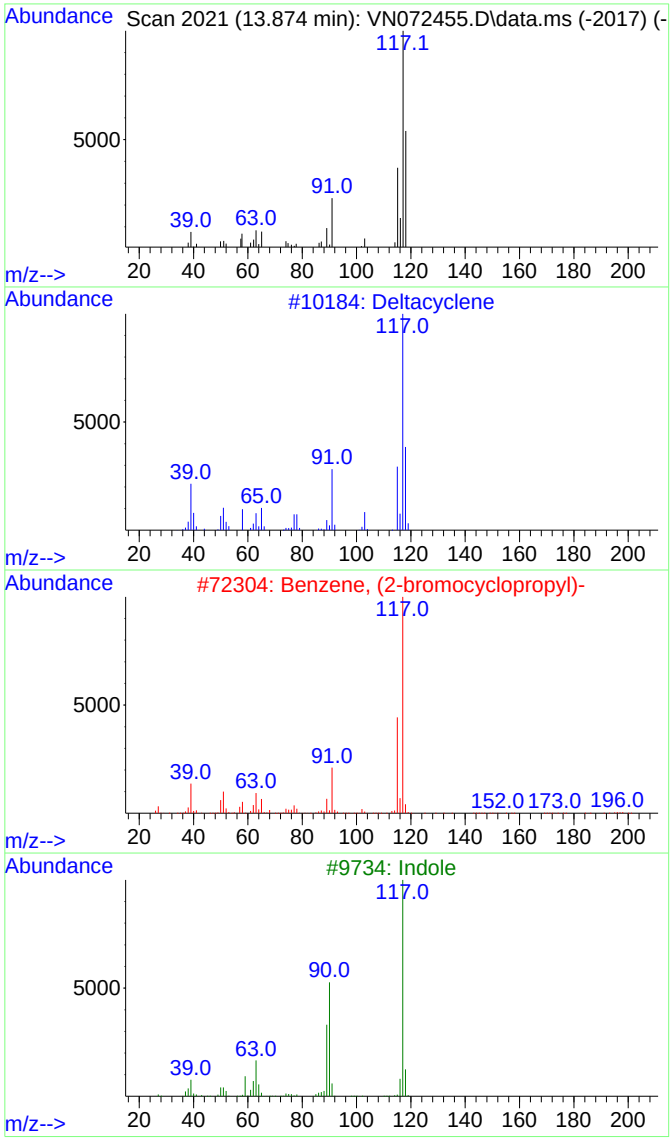
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

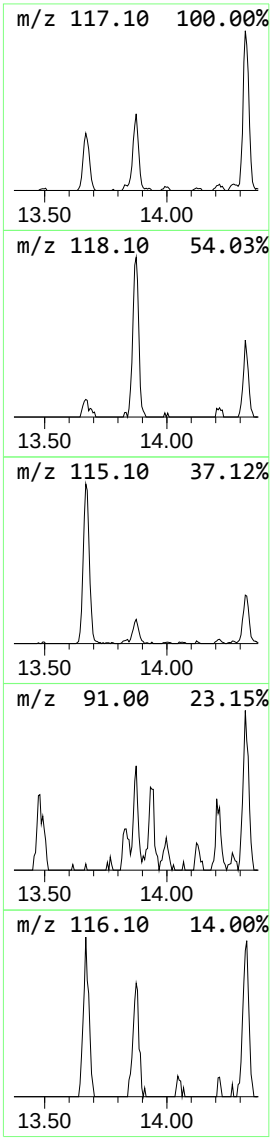
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, (2-bromocyclopropyl)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	5.86 ug/l	70393	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Deltacyclene	118	C9H10	007785-10-6	59
2	Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	53
3	Indole	117	C8H7N	000120-72-9	47
4	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	45
5	m-Aminophenylacetylene	117	C8H7N	054060-30-9	43





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Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

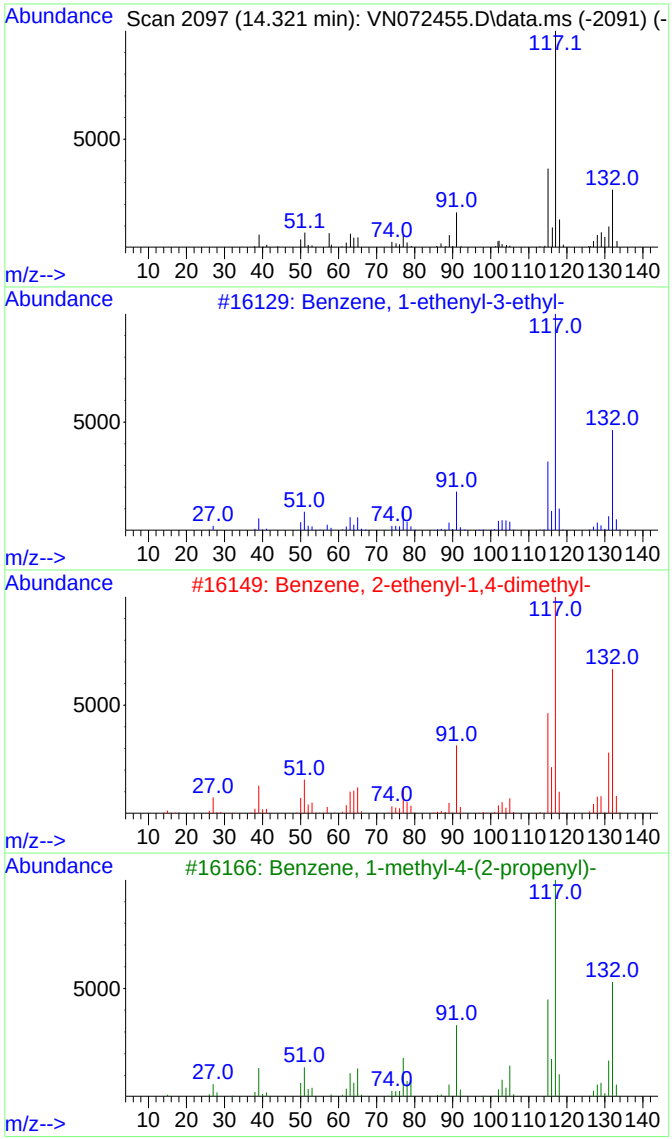
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

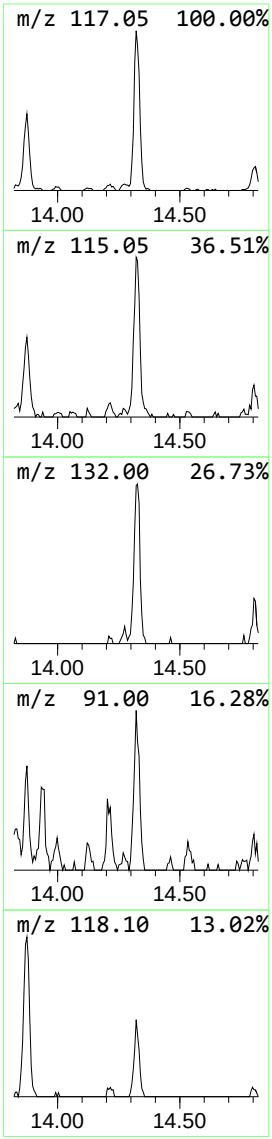
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.321	12.02 ug/l	144371	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	87
3	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
Acq On : 12 May 2022 16:08
Operator : JC\MD
Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

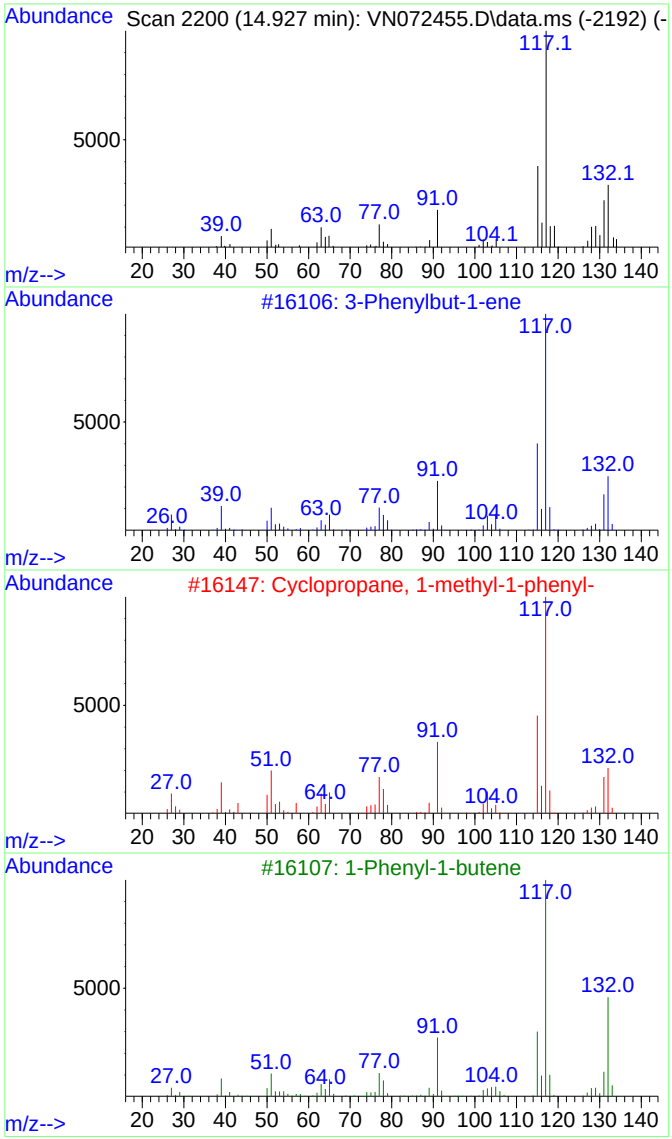
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Quant Title : SW846 8260

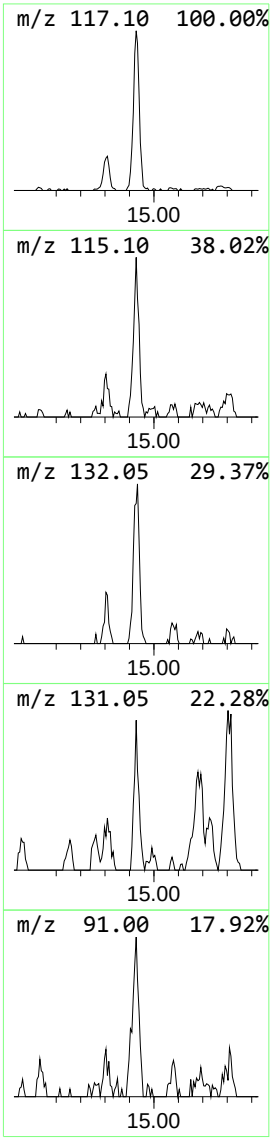
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Phenylbut-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	11.87 ug/l	142661	1,4-Dichlorobenzene-d4	13.668

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
2	Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	81
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	68
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	68
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072455.D
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Sample : N2800-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.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
Butane, 2-methyl-	3.122	24.9	ug/l	293449	1	8.086	589701	50.0
Butane, 2,3-dim...	5.081	18.5	ug/l	218551	1	8.086	589701	50.0
Pentane, 3-methyl-	5.616	22.9	ug/l	270339	1	8.086	589701	50.0
Pentane, 2,3-di...	8.175	9.2	ug/l	107991	1	8.086	589701	50.0
Benzene, (2-bro...	13.874	5.9	ug/l	70393	4	13.668	600760	50.0
Benzene, 1-ethe...	14.321	12.0	ug/l	144371	4	13.668	600760	50.0
3-Phenylbut-1-ene	14.927	11.9	ug/l	142661	4	13.668	600760	50.0