

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
 Data File : VY019172.D
 Acq On : 21 Aug 2024 16:17
 Operator : SY/MD
 Sample : P3641-08
 Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 S-910-K1-0-0.5-081524-FD

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_Y\methods\82Y081524S.M
 Title : SW846 8260

Signal : TIC: VY019172.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.610	464	474	484	rBV4	7056	19437	3.72%	0.517%
2	5.634	636	642	649	rBV5	2057	6095	1.17%	0.162%
3	7.628	958	969	975	rBV	77201	187177	35.78%	4.983%
4	7.701	975	981	992	rVB	133396	307102	58.71%	8.176%
5	8.055	1027	1039	1049	rBV2	58661	131732	25.18%	3.507%
6	8.609	1121	1130	1141	rBV	202488	405281	77.48%	10.790%
7	10.103	1365	1375	1385	rBV	305276	523081	100.00%	13.926%
8	10.505	1435	1441	1450	rVB4	2301	5240	1.00%	0.140%
9	11.414	1582	1590	1599	rBV	259564	434277	83.02%	11.562%
10	11.530	1602	1609	1610	rBV5	3888	6943	1.33%	0.185%
11	12.261	1724	1729	1733	rVB4	4796	7080	1.35%	0.188%
12	12.408	1743	1753	1762	rBV2	182453	319297	61.04%	8.501%
13	12.511	1766	1770	1777	rVB7	2710	5594	1.07%	0.149%
14	13.042	1838	1857	1868	rBV7	45793	245237	46.88%	6.529%
15	13.346	1901	1907	1914	rVB	192583	300585	57.46%	8.003%
16	13.462	1915	1926	1936	rVB	7263	28095	5.37%	0.748%
17	13.609	1938	1950	1954	rBV5	43094	154005	29.44%	4.100%
18	13.712	1962	1967	1980	rVB6	45181	153769	29.40%	4.094%
19	13.828	1982	1986	1991	rVB8	3294	5478	1.05%	0.146%
20	13.889	1991	1996	2002	rBV	44022	66708	12.75%	1.776%
21	14.078	2016	2027	2050	rVB6	50375	277813	53.11%	7.396%
22	14.304	2057	2064	2073	rBV8	10634	31254	5.97%	0.832%
23	14.425	2073	2084	2090	rBV4	16410	59424	11.36%	1.582%
24	14.499	2092	2096	2102	rVB5	9468	23654	4.52%	0.630%
25	14.944	2160	2169	2180	rBV2	19285	45591	8.72%	1.214%
26	15.584	2267	2274	2280	rBV7	2578	6085	1.16%	0.162%

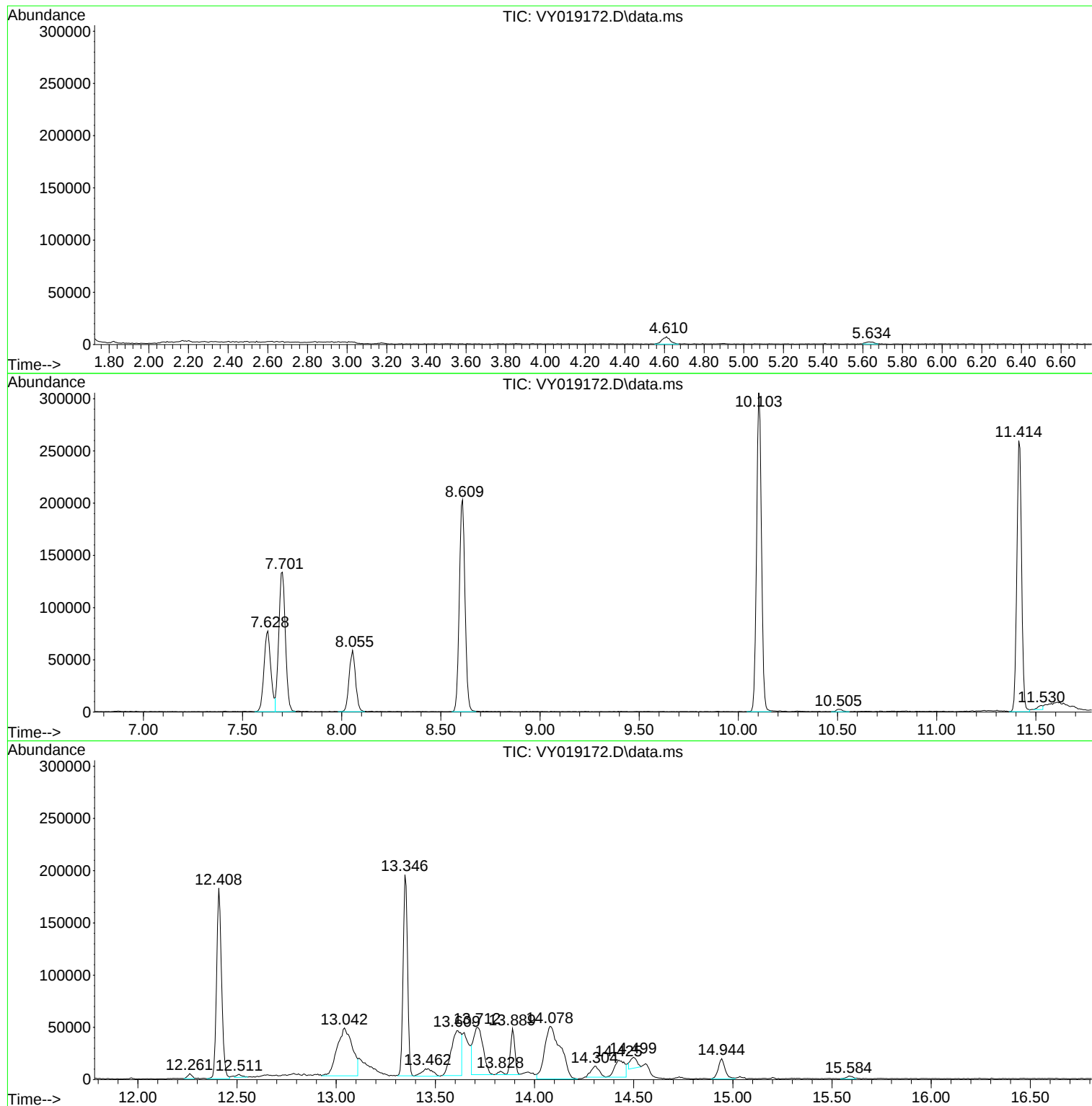
Sum of corrected areas: 3756034

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

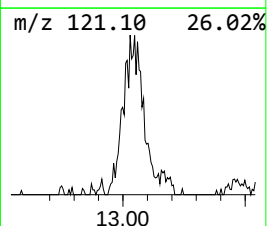
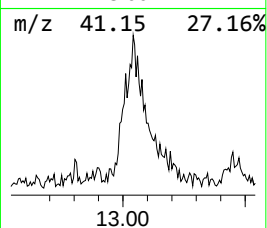
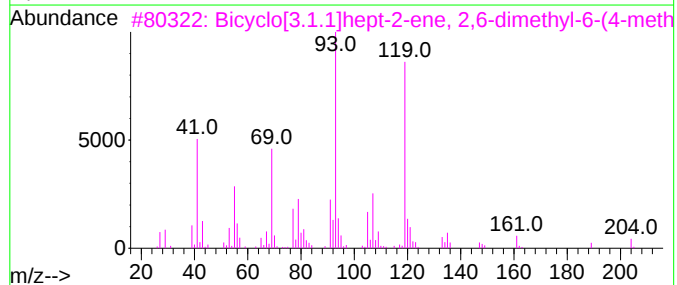
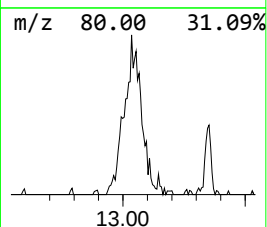
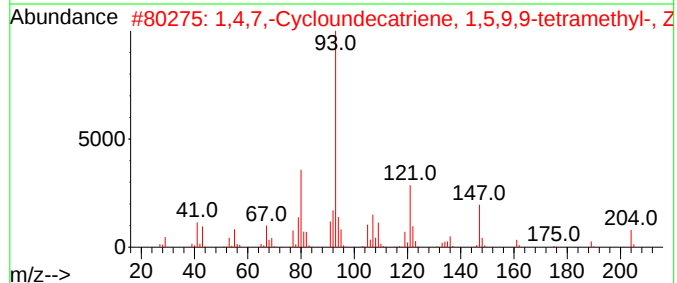
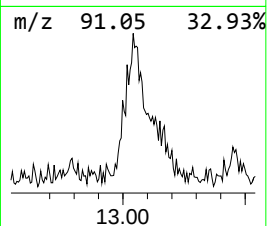
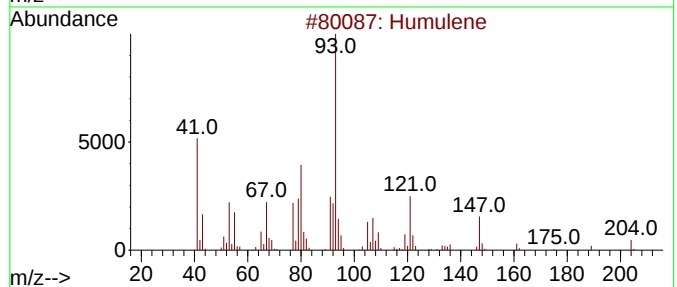
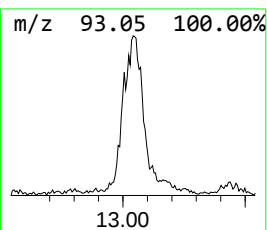
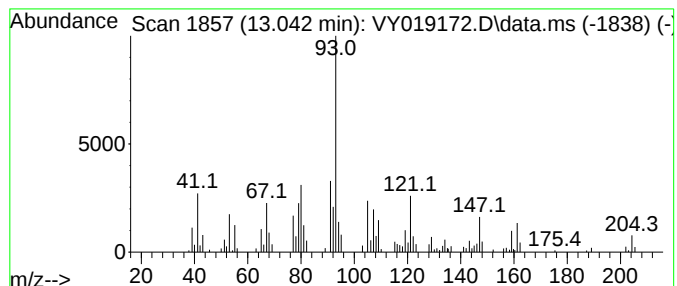
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 1 Humulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.042	40.79 ug/l	245237	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Humulene	204	C15H24	006753-98-6	98
2			1,4,7,-Cycloundecatriene, 1,5,9,...	204	C15H24	1000062-61-9	89
3			Bicyclo[3.1.1]hept-2-ene, 2,6-di...	204	C15H24	017699-05-7	53
4			1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	53
5			trans-.beta.-Ocimene	136	C10H16	003779-61-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

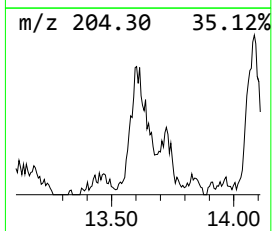
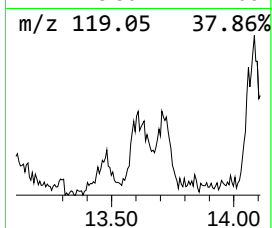
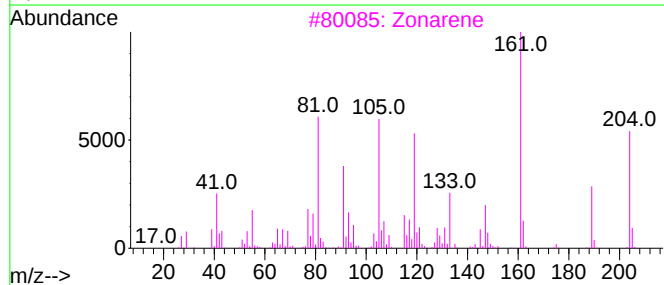
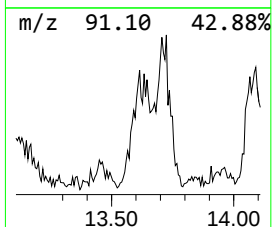
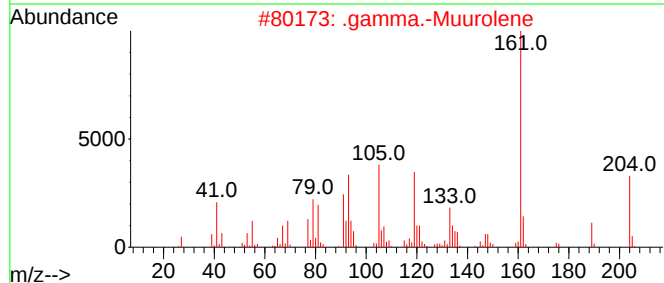
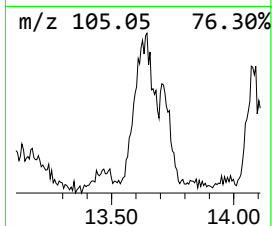
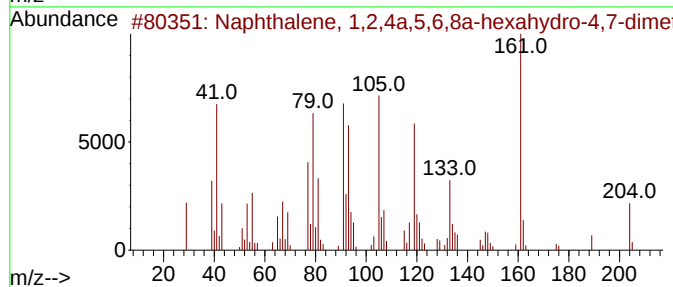
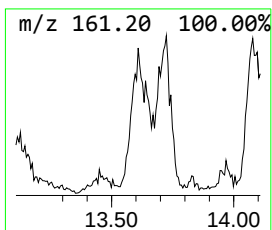
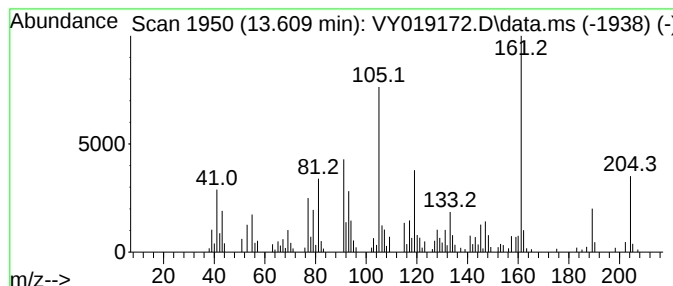
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 2 Naphthalene, 1,2,4a,5,6,8a-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.608	25.62 ug/l	154005	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,4a,5,6,8a-hexah...	204	C15H24	000483-75-0	95
2			.gamma.-Muurolene	204	C15H24	030021-74-0	95
3			Zonarene	204	C15H24	041929-05-9	93
4			Cyclohexene, 6-ethenyl-6-methyl-...	204	C15H24	005951-67-7	93
5			Azulene, 1,2,3,3a,4,5,6,7-octahy...	204	C15H24	022567-17-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

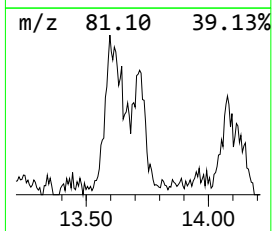
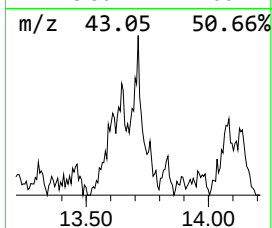
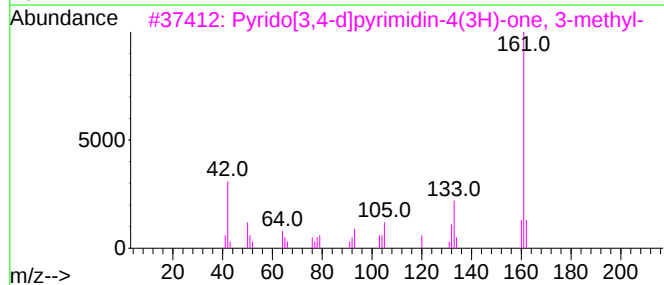
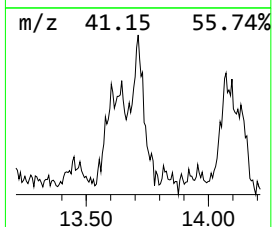
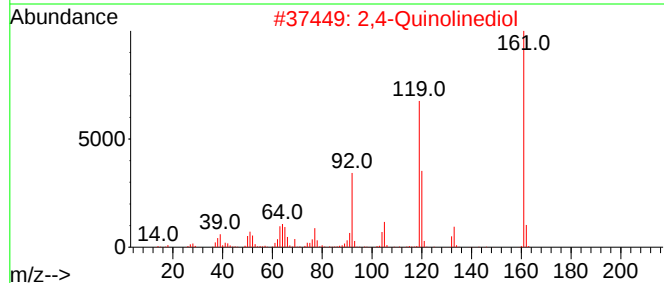
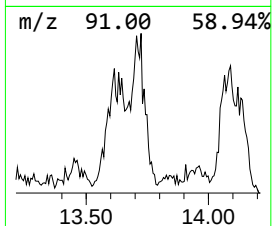
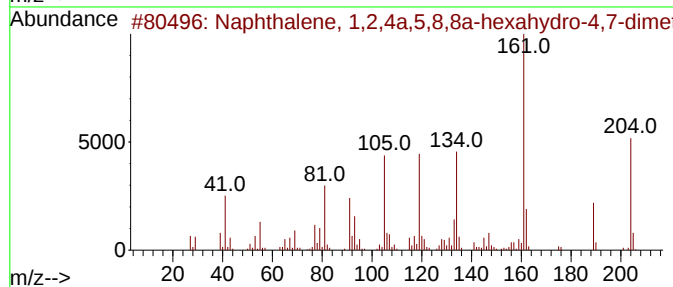
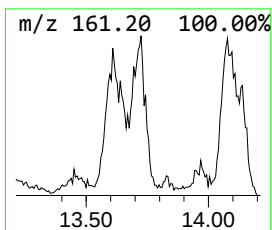
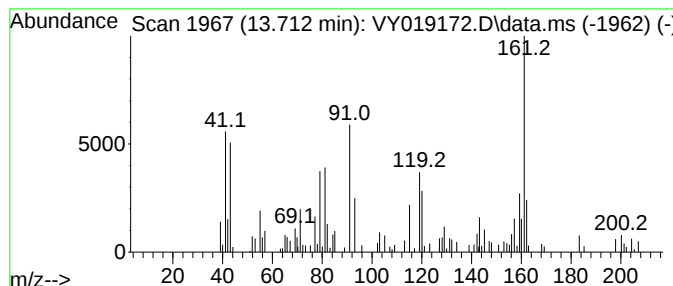
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 1,2,4a,5,8,8a-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.712	25.58 ug/l	153769	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	50
2			2,4-Quinolinediol	161	C9H7NO2	000086-95-3	50
3			Pyrido[3,4-d]pyrimidin-4(3H)-one...	161	C8H7N3O	022389-82-8	43
4			2-(3-Isobutylphenyl)propionic acid	206	C13H18O2	066622-47-7	40
5			1H-Cyclopenta[1,3]cyclopropa[1,2...	204	C15H24	013744-15-5	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

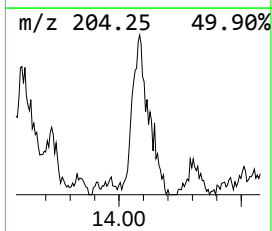
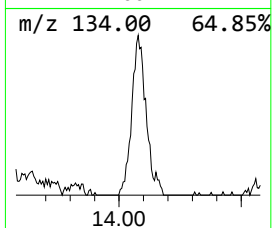
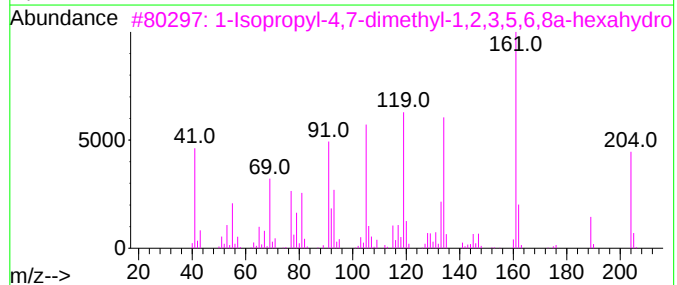
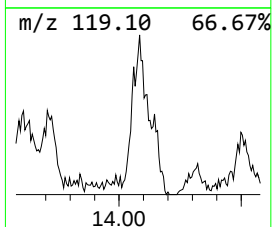
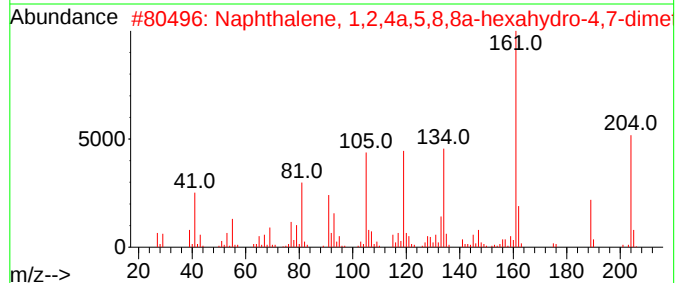
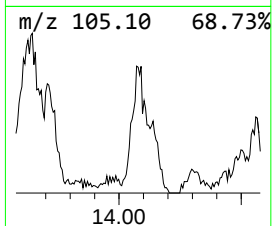
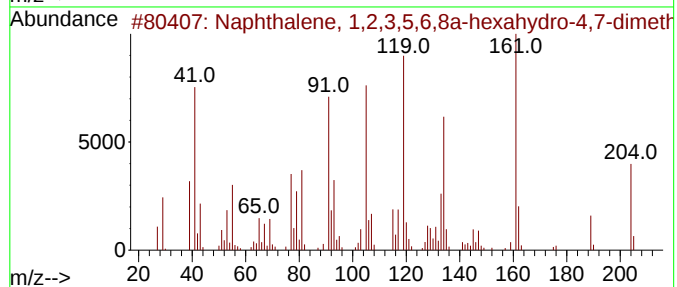
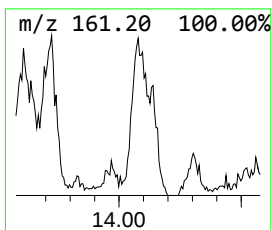
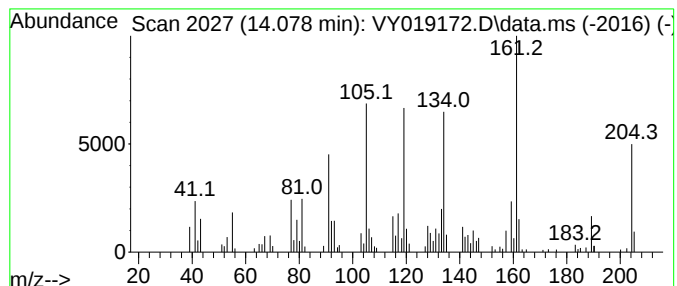
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.078	46.21 ug/l	277813	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	94
2			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	93
3			1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	91
4			Epizonarene	204	C15H24	041702-63-0	89
5			Zonarene	204	C15H24	041929-05-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

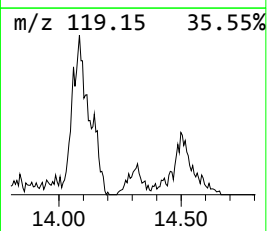
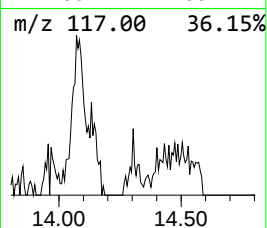
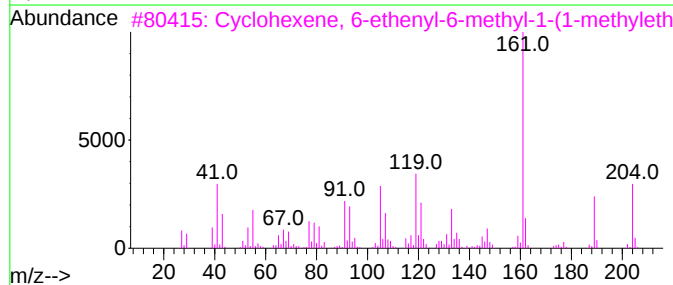
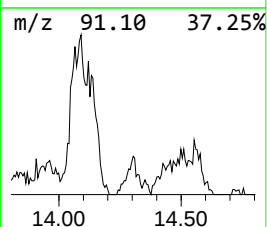
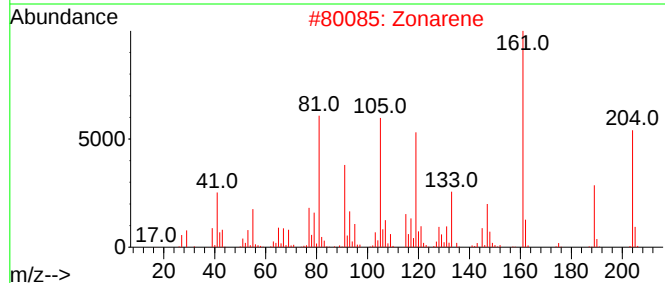
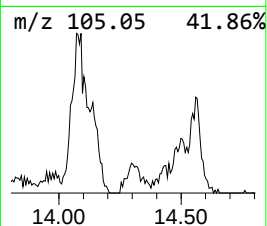
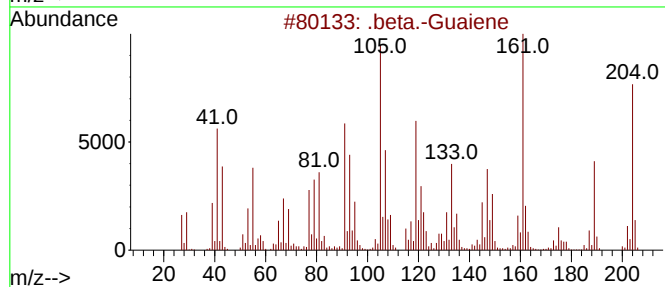
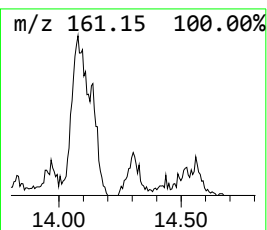
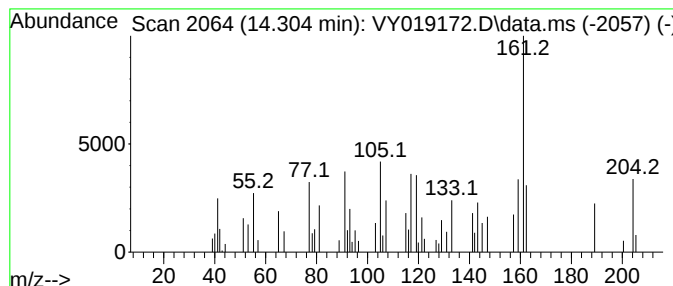
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 6 .beta.-Guaiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.304	5.20 ug/l	31254	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Guaiene	204	C15H24	000088-84-6	87
2			Zonarene	204	C15H24	041929-05-9	70
3			Cyclohexene, 6-ethenyl-6-methyl-...	204	C15H24	005951-67-7	70
4			Azulene, 1,2,3,3a,4,5,6,7-octahy...	204	C15H24	022567-17-5	68
5			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

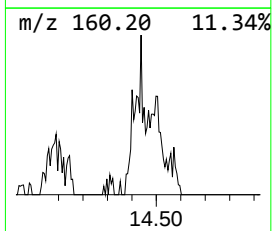
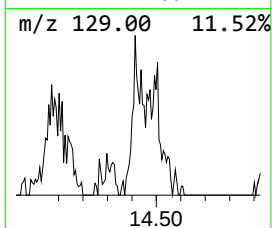
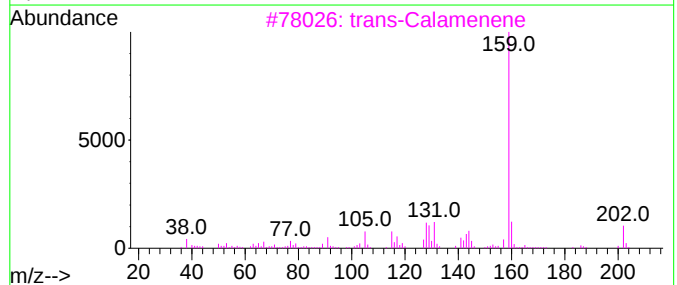
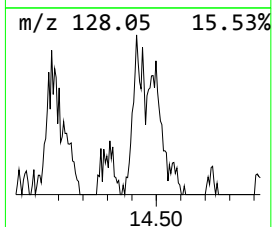
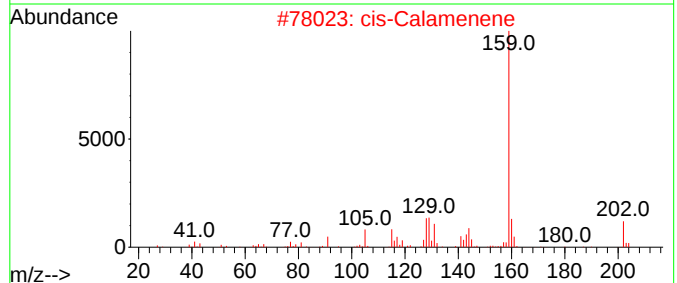
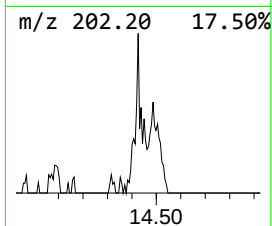
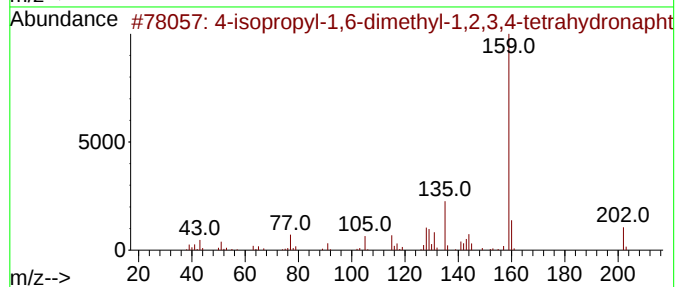
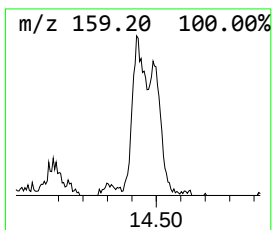
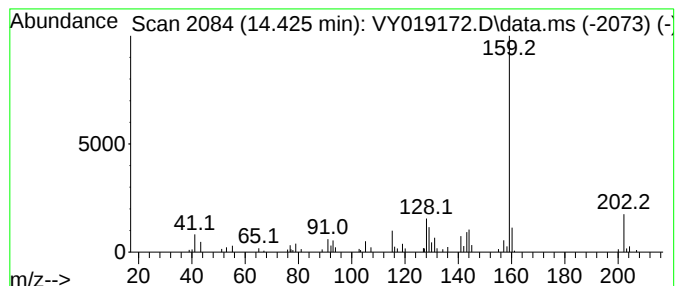
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 7 4-isopropyl-1,6-dimethyl-1,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.426	9.88 ug/l	59424	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-isopropyl-1,6-dimethyl-1,2,3,4...	202	C15H22	1000378-99-6	94
2			cis-Calamenene	202	C15H22	072937-55-4	91
3			trans-Calamenene	202	C15H22	073209-42-4	91
4			Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	86
5			Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

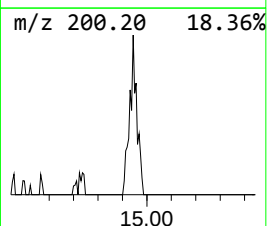
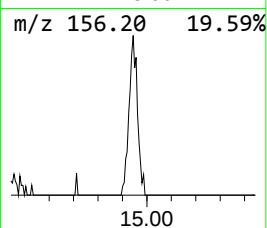
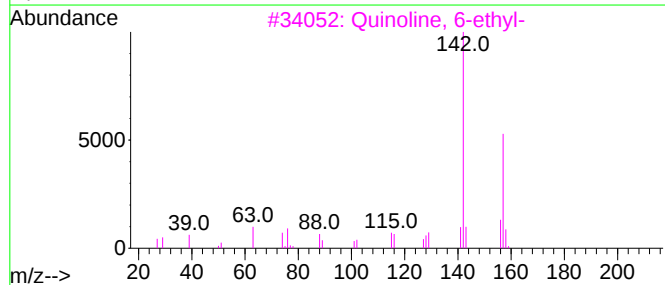
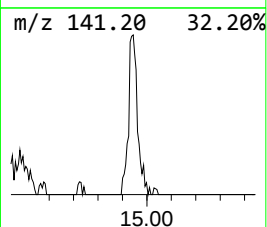
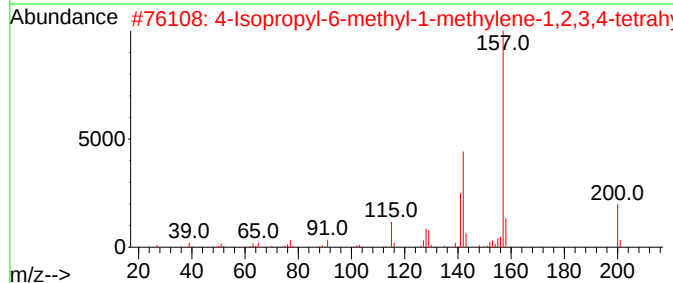
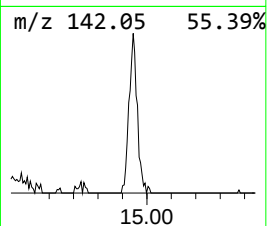
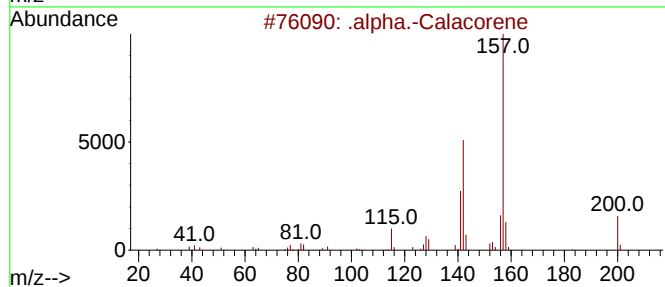
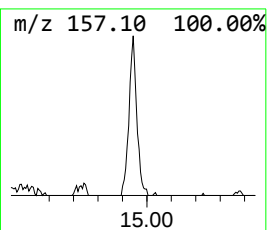
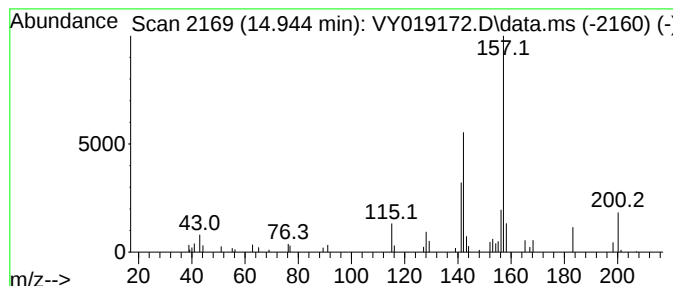
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.M
Quant Title : SW846 8260

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

Peak Number 8 .alpha.-Calacorene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.944	7.58 ug/l	45591	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Calacorene	200	C15H20	021391-99-1	95
2			4-Isopropyl-6-methyl-1-methylene...	200	C15H20	050277-34-4	90
3			Quinoline, 6-ethyl-	157	C11H11N	019655-60-8	53
4			Quinoline, 3-ethyl-	157	C11H11N	001873-54-7	53
5			Pyrimidine, 5-chloro-2-dimethyla...	157	C6H8ClN3	081568-09-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY082124\
Data File : VY019172.D
Acq On : 21 Aug 2024 16:17
Operator : SY/MD
Sample : P3641-08
Misc : 5.13g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-910-K1-0-0.5-081524-FD

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y081524S.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
Humulene	13.042	40.8	ug/l	245237	4	13.346	300585	50.0
Naphthalene, 1,...	13.608	25.6	ug/l	154005	4	13.346	300585	50.0
Naphthalene, 1,...	13.712	25.6	ug/l	153769	4	13.346	300585	50.0
Naphthalene, 1,...	14.078	46.2	ug/l	277813	4	13.346	300585	50.0
.beta.-Guaiene	14.304	5.2	ug/l	31254	4	13.346	300585	50.0
4-isopropyl-1,6...	14.426	9.9	ug/l	59424	4	13.346	300585	50.0
.alpha.-Calacorene	14.944	7.6	ug/l	45591	4	13.346	300585	50.0