LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\Method\SFAMUTR012725WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU063051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.618	95	102	119	rVB2	86827	151151	1.20%	0.527%
2	5.087	1164	1181	1197	rBV	59646	136611	1.09%	0.476%
3	5.769	1376	1393	1417	rBV2	113425	278632	2.22%	0.971%
4	6.283	1541	1553	1574	rVB	133677	254688	2.03%	0.888%
5	7.907	2047	2058	2074	rBV	141656	241600	1.92%	0.842%
6	8.643	2275	2287	2309	rBV	130970	231142	1.84%	0.806%
7	9.415	2516	2527	2542	rBV	200548	327060	2.60%	1.140%
8	11.804	3259	3270	3295	rVB	274550	458212	3.64%	1.598%
9	12.049	3319	3346	3379	rBV	7690936	12574178	100.00%	43.839%
10	12.184	3380	3388	3410	rVB	240826	471320	3.75%	1.643%
11	13.254	3713	3721	3733	rBV	221069	335640	2.67%	1.170%
12	14.074	3971	3976	3985	rVB	241050	345974	2.75%	1.206%
13	14.412	4072	4081	4125	rVB	999924	2008244	15.97%	7.002%
14	15.100	4286	4295	4308	rVB	443450	696123	5.54%	2.427%
15	15.476	4400	4412	4436	rBV	749543	1486514	11.82%	5.183%
16	15.708	4476	4484	4496	rVB	318354	480114	3.82%	1.674%
17	16.225	4633	4645	4677	rBV	4157666	7333349	58.32%	25.567%
18	16.479	4716	4724	4753	rVB	443661	871977	6.93%	3.040%

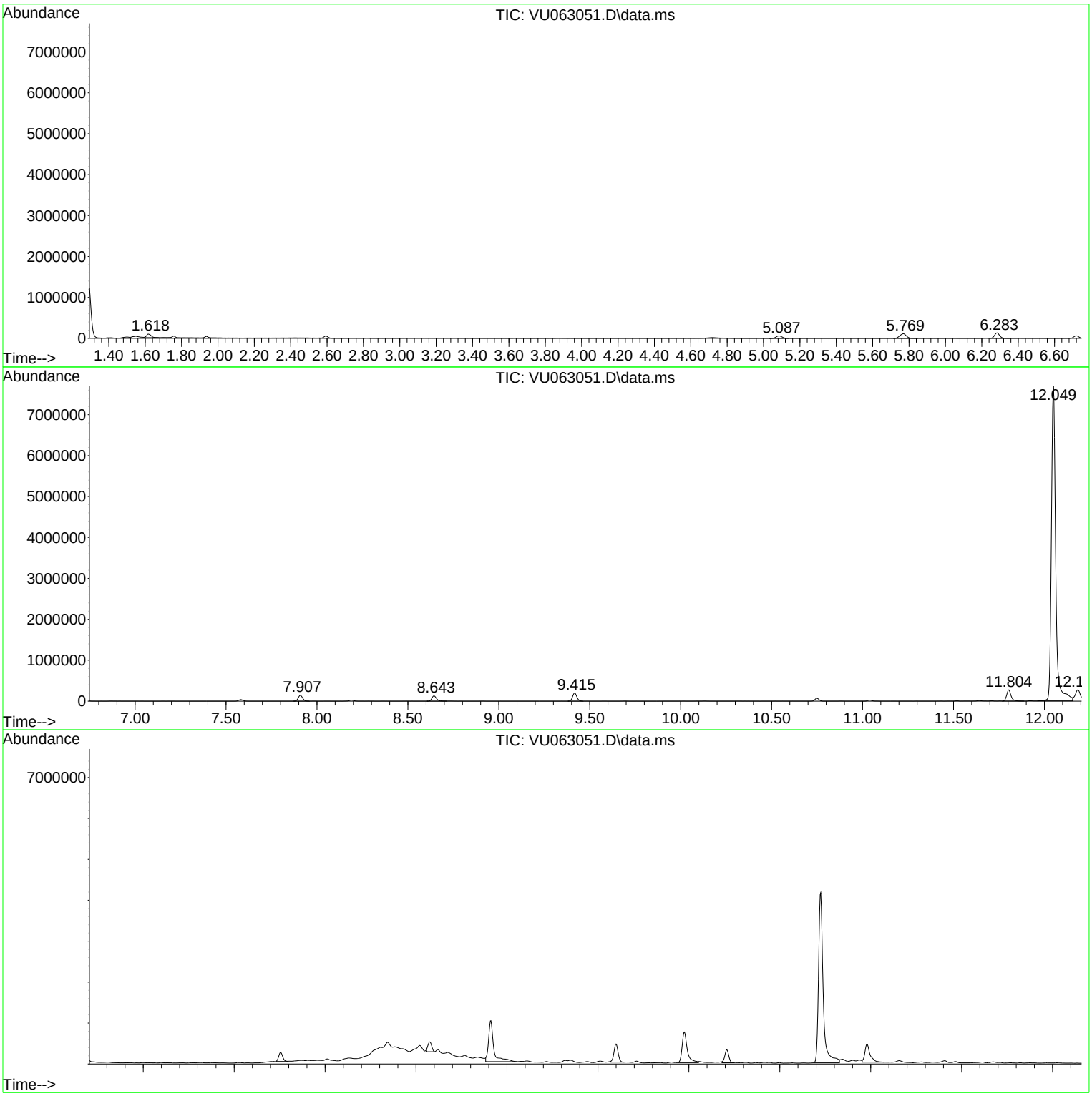
Sum of corrected areas: 28682529

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

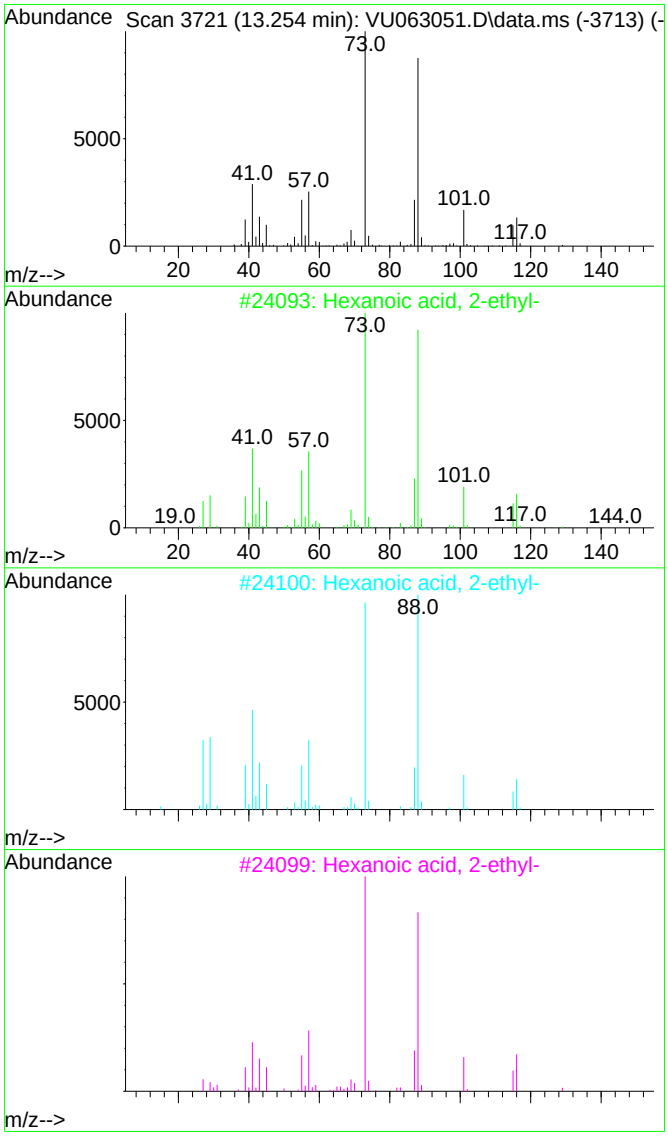
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

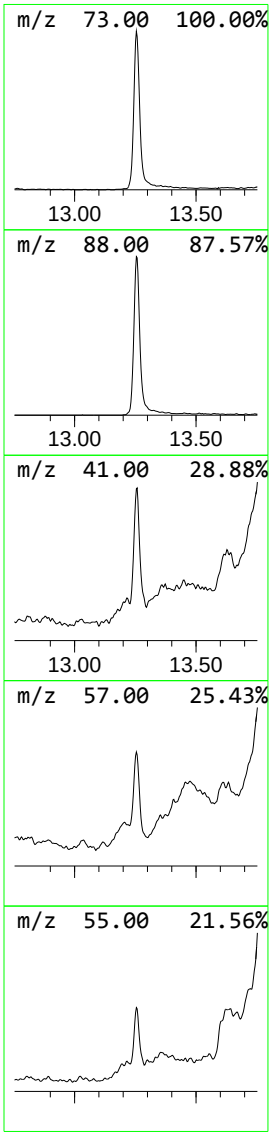
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.254	3.66 ug/L	335640	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	91
2	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

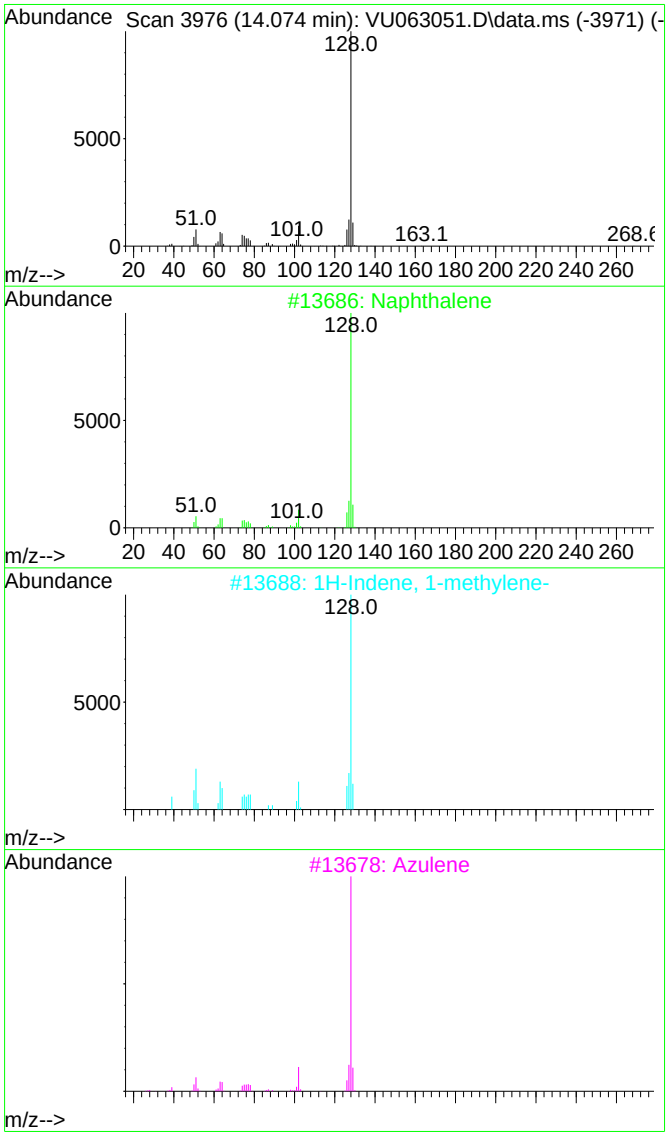
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

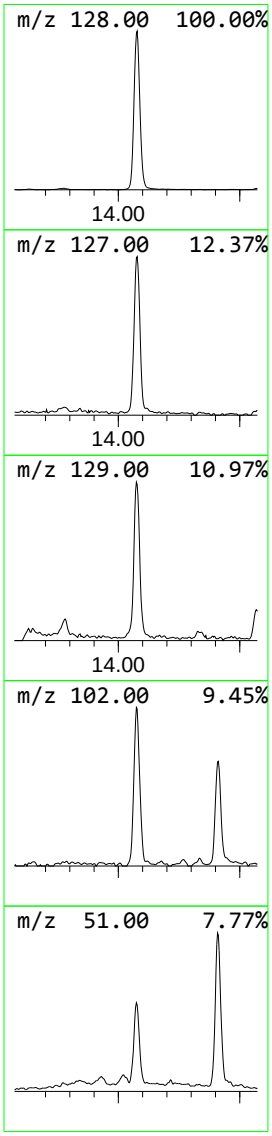
****

Peak Number 3 Azulene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	3.78 ug/L	345974	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	95
2	1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3	Azulene	128	C10H8	000275-51-4	94
4	Naphthalene	128	C10H8	000091-20-3	94
5	Azulene	128	C10H8	000275-51-4	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

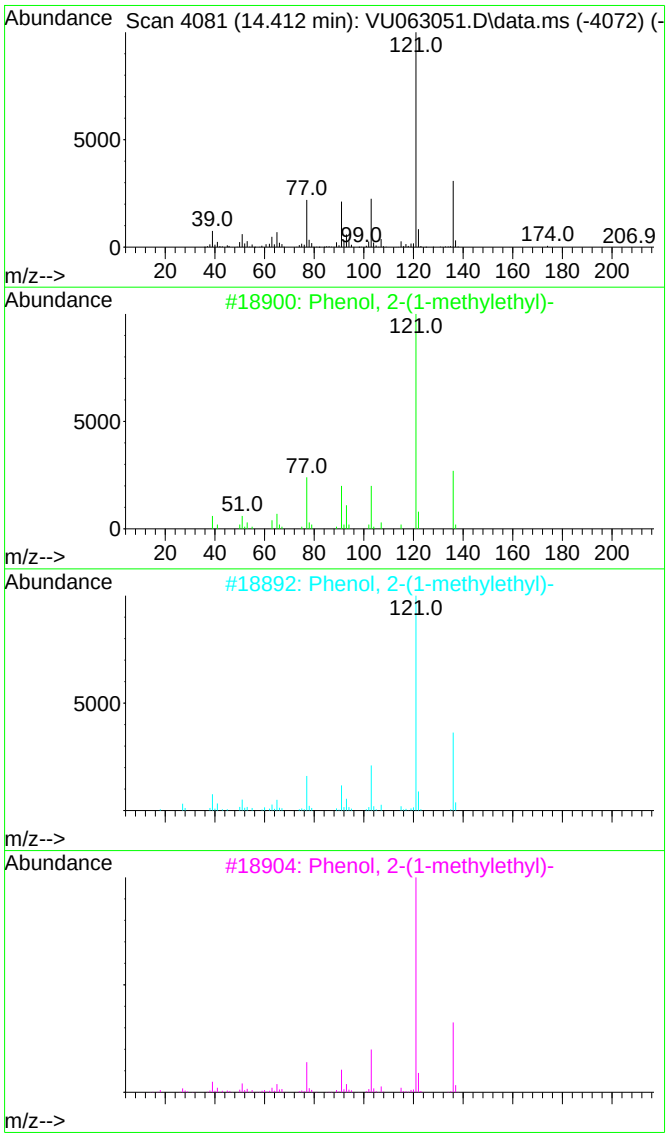
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

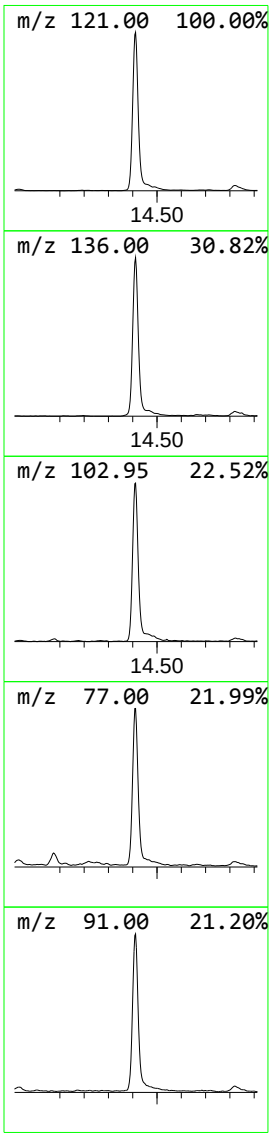
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 2-(1-methylethyl)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.412	21.91 ug/L	2008240	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	94
2	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	93
3	Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
4	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90
5	Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

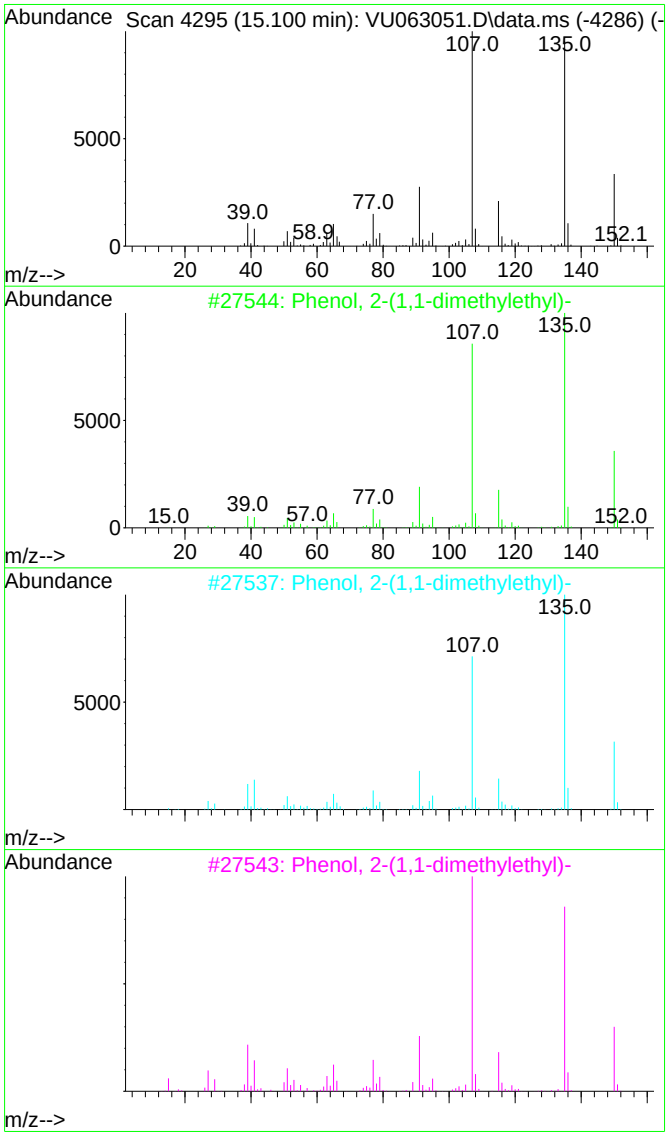
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

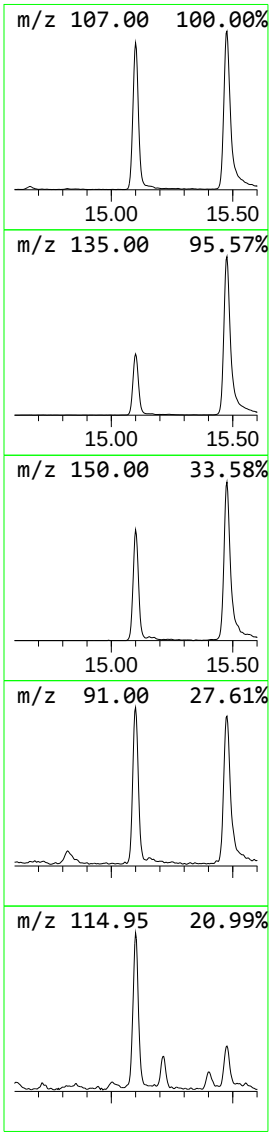
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 2-(1,1-dimethylethyl)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.100	7.60 ug/L	696123	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	96
2	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	93
3	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	000088-18-6	93
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

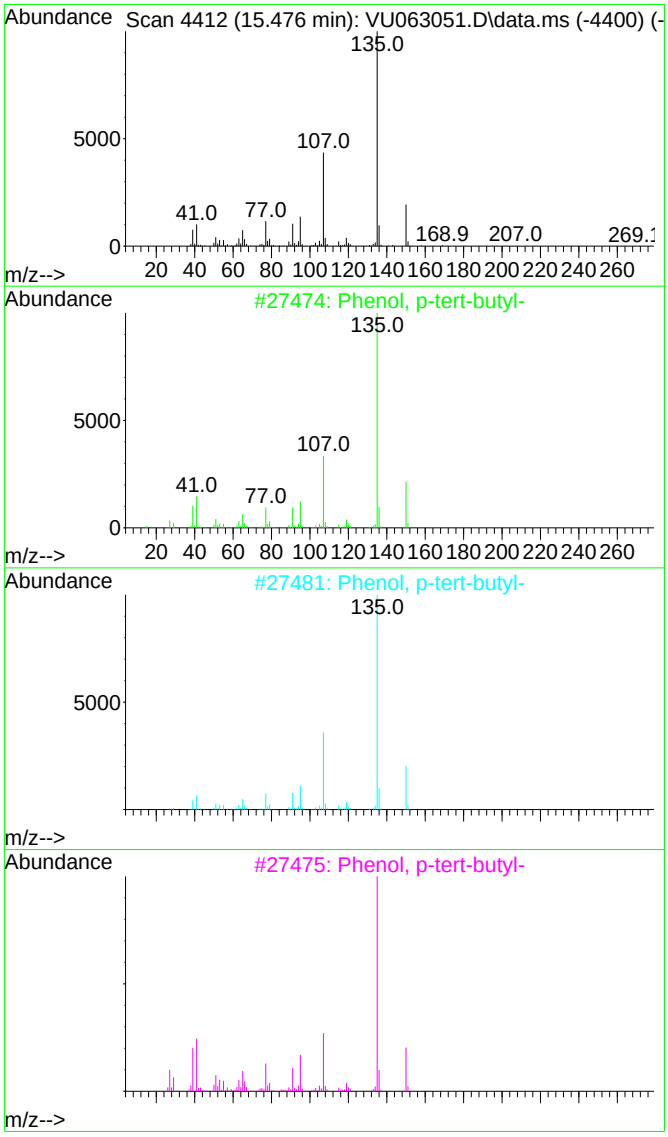
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

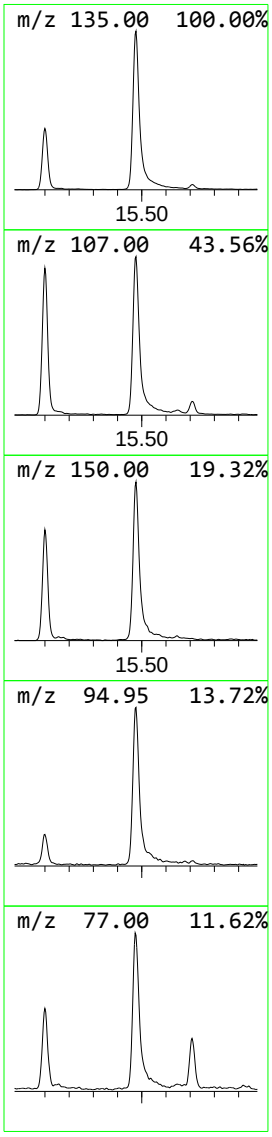
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenol, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.476	16.22 ug/L	1486510	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	96
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	94
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	94
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	93





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

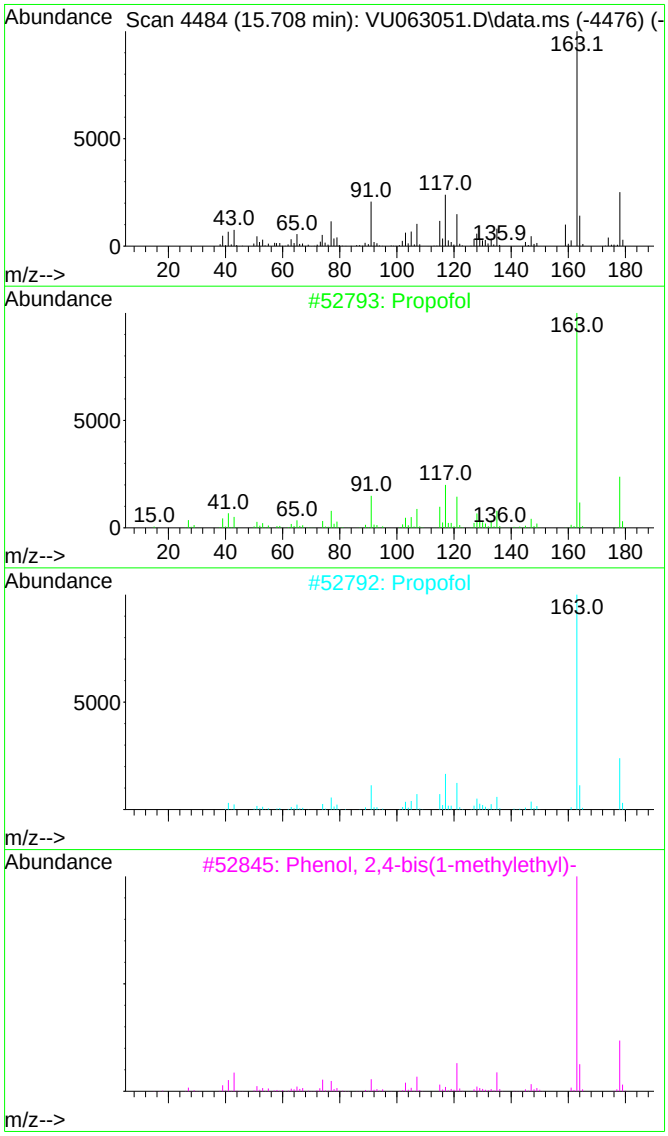
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

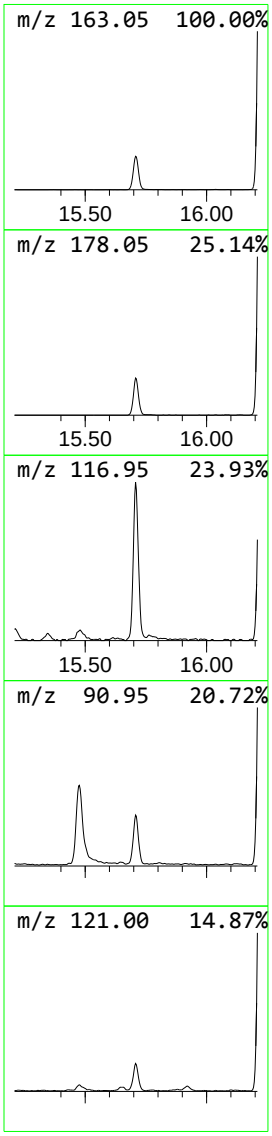
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propofol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.708	5.24 ug/L	480114	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propofol	178	C12H18O	002078-54-8	96
2	Propofol	178	C12H18O	002078-54-8	94
3	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	93
4	Propofol	178	C12H18O	002078-54-8	93
5	Propofol	178	C12H18O	002078-54-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

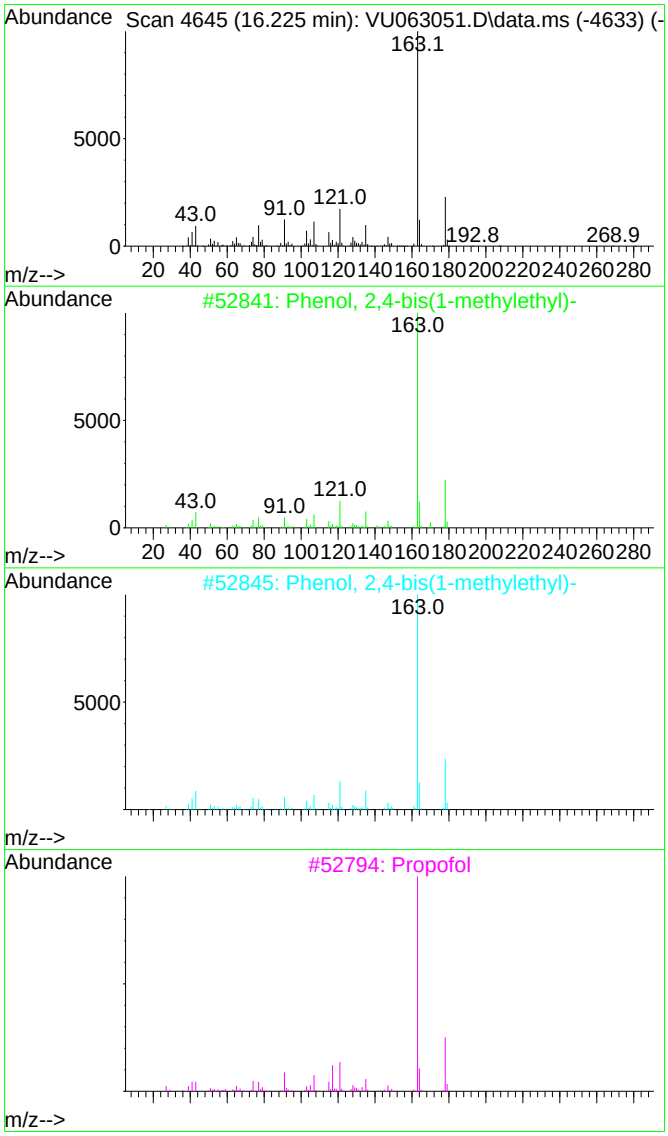
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

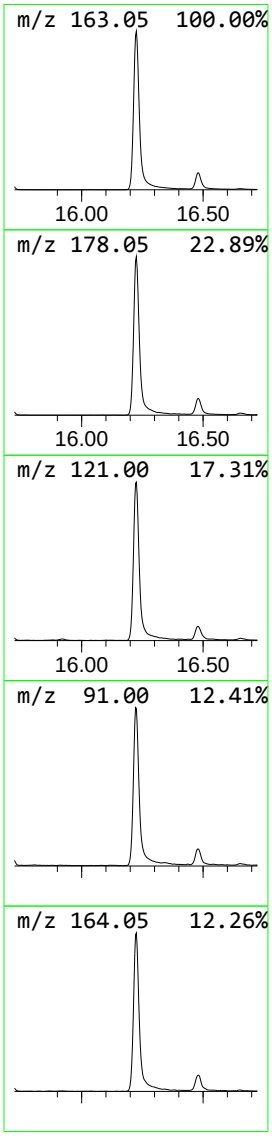
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Phenol, 2,4-bis(1-methyleth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.225	80.02 ug/L	7333350	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	95
2	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	95
3	Propofol	178	C12H18O	002078-54-8	93
4	Propofol	178	C12H18O	002078-54-8	91
5	Propofol	178	C12H18O	002078-54-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
Sample : Q1195-16
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E2967

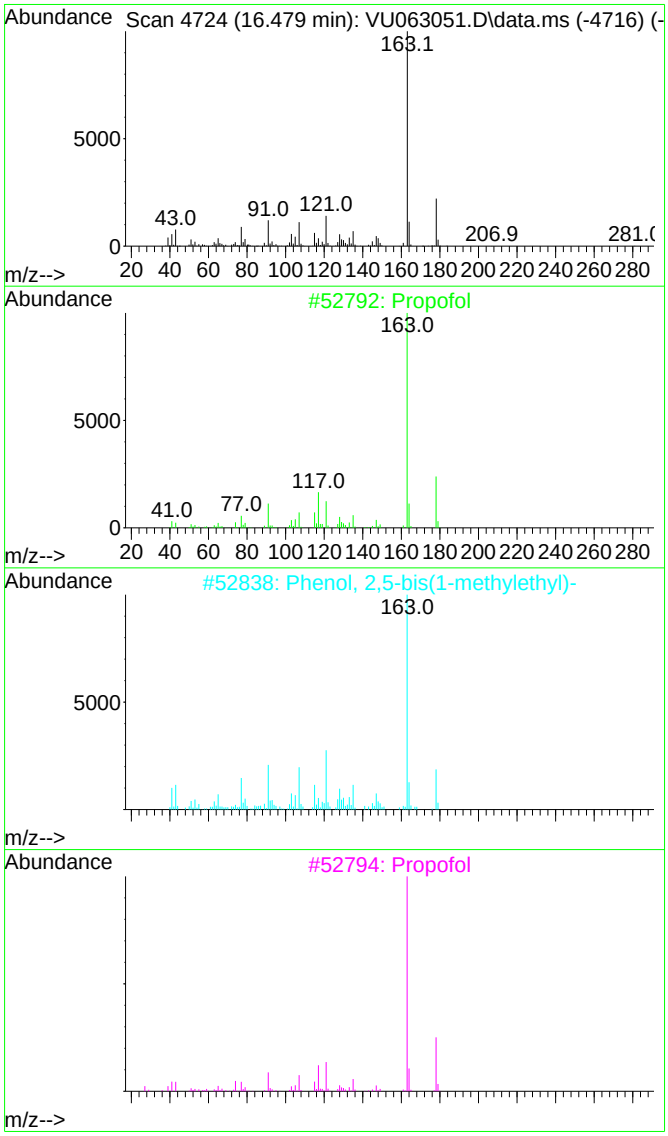
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

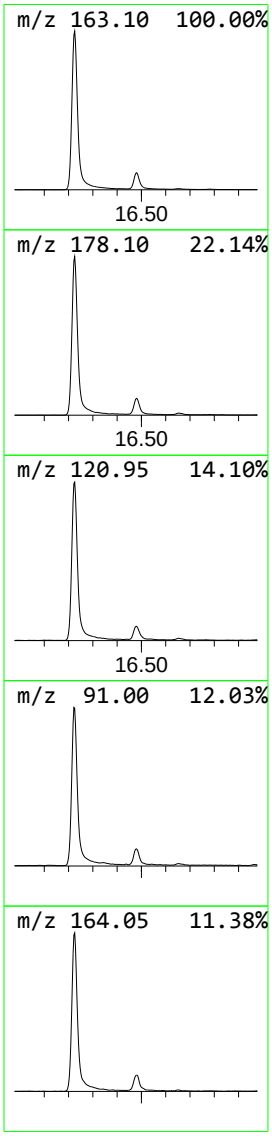
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Phenol, 2,5-bis(1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.479	9.52 ug/L	871977	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propofol	178	C12H18O	002078-54-8	94
2	Phenol, 2,5-bis(1-methylethyl)-	178	C12H18O	035946-91-9	94
3	Propofol	178	C12H18O	002078-54-8	93
4	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	90
5	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012725\
Data File : VU063051.D
Acq On : 28 Jan 2025 06:31
Operator : MD/SY
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Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012725WMA.M
Quant Title : TRACE VOA SFAM1.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hexanoic acid, ...	13.254	3.7	ug/L	335640	3	11.804	458212	5.0
Azulene	14.074	3.8	ug/L	345974	3	11.804	458212	5.0
Phenol, 2-(1-me...	14.412	21.9	ug/L	2008240	3	11.804	458212	5.0
Phenol, 2-(1,1-...	15.100	7.6	ug/L	696123	3	11.804	458212	5.0
Phenol, p-tert-...	15.476	16.2	ug/L	1486510	3	11.804	458212	5.0
Propofol	15.708	5.2	ug/L	480114	3	11.804	458212	5.0
Phenol, 2,4-bis...	16.225	80.0	ug/L	7333350	3	11.804	458212	5.0
Phenol, 2,5-bis...	16.479	9.5	ug/L	871977	3	11.804	458212	5.0