

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110424\
 Data File : BP022868.D
 Acq On : 05 Nov 2024 20:14
 Operator : RC/JU
 Sample : P4670-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0SY5

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP022868.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.046	334	350	354	rBV2	30276478	100388321	95.29%	24.760%
2	6.828	646	653	667	rVB2	104652	253252	0.24%	0.062%
3	6.981	671	679	689	rBV	205024	366390	0.35%	0.090%
4	7.175	705	712	728	rBV	301061	568310	0.54%	0.140%
5	7.528	762	772	783	rBV	7959170	15504523	14.72%	3.824%
6	7.710	783	803	807	rBV	29048402	91994833	87.32%	22.690%
7	8.040	841	859	863	rBV	28698790	105353631	100.00%	25.985%
8	8.340	903	910	924	rBV	182988	341689	0.32%	0.084%
9	8.769	976	983	987	rBV	320300	571244	0.54%	0.141%
10	8.816	987	991	1000	rVB	502962	820522	0.78%	0.202%
11	9.099	1032	1039	1048	rBV	176284	292668	0.28%	0.072%
12	9.410	1087	1092	1098	rVB	89560	166850	0.16%	0.041%
13	9.481	1098	1104	1112	rBV	310048	575906	0.55%	0.142%
14	10.028	1187	1197	1205	rBV	444592	757644	0.72%	0.187%
15	10.275	1227	1239	1244	rBV	23299618	48539346	46.07%	11.972%
16	10.387	1252	1258	1265	rVB	387827	605867	0.58%	0.149%
17	10.775	1312	1324	1340	rBV	6078612	11274495	10.70%	2.781%
18	10.981	1352	1359	1376	rVB	355860	631447	0.60%	0.156%
19	11.198	1389	1396	1405	rBV2	172575	308505	0.29%	0.076%
20	12.416	1598	1603	1611	rVB	694718	1071129	1.02%	0.264%
21	13.028	1699	1707	1719	rBV	1852443	3002087	2.85%	0.740%
22	13.651	1802	1813	1818	rBV	792976	1186628	1.13%	0.293%
23	13.698	1818	1821	1842	rVB5	41735	121148	0.11%	0.030%
24	13.934	1853	1861	1870	rBV	882543	1250564	1.19%	0.308%
25	14.239	1905	1913	1921	rBV	613872	973550	0.92%	0.240%
26	14.510	1952	1959	1964	rBV2	85318	198754	0.19%	0.049%
27	14.563	1964	1968	1982	rVB2	75362	149017	0.14%	0.037%
28	15.251	2077	2085	2091	rBV	1210584	1797562	1.71%	0.443%
29	15.310	2091	2095	2102	rVV	89150	148474	0.14%	0.037%
30	15.392	2102	2109	2122	rVV	408598	588954	0.56%	0.145%
31	16.545	2295	2305	2314	rBV	112490	238393	0.23%	0.059%
32	17.051	2385	2391	2400	rBV	1016339	1333476	1.27%	0.329%
33	17.145	2400	2407	2419	rVB2	1482598	2034923	1.93%	0.502%
34	17.992	2546	2551	2559	rBV	239086	369831	0.35%	0.091%
35	18.480	2626	2634	2642	rBV2	195613	307623	0.29%	0.076%
36	18.980	2711	2719	2724	rBV	77717	126496	0.12%	0.031%

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ClientSampleId :
C0SY5

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Title : SVOA CALIBRATION

37	19.327	2772	2778	2789	rBV	350908	522774	0.50%	0.129%
38	19.533	2807	2813	2822	rBV	1969007	2847485	2.70%	0.702%
39	21.492	3140	3146	3155	rBV	1196412	1812352	1.72%	0.447%
40	21.621	3164	3168	3174	rVB	257213	357839	0.34%	0.088%
41	24.533	3654	3663	3676	rVB	1279587	3268301	3.10%	0.806%
42	24.751	3690	3700	3711	rVB2	642820	1857941	1.76%	0.458%
43	25.280	3783	3790	3801	rVB	258428	558862	0.53%	0.138%

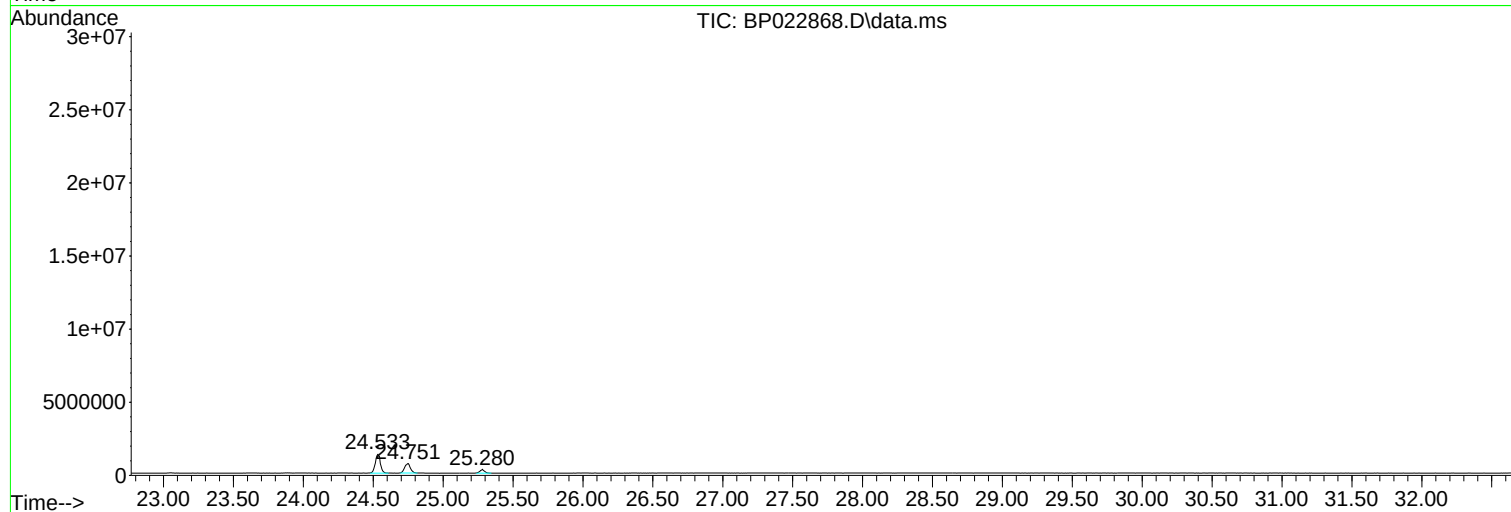
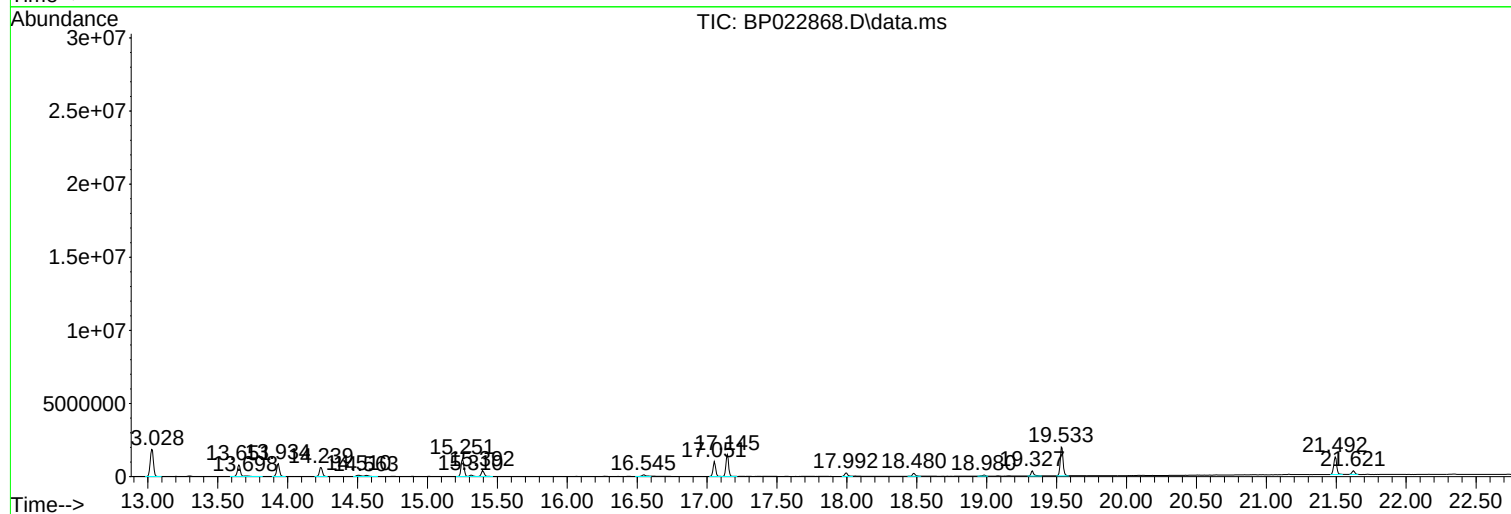
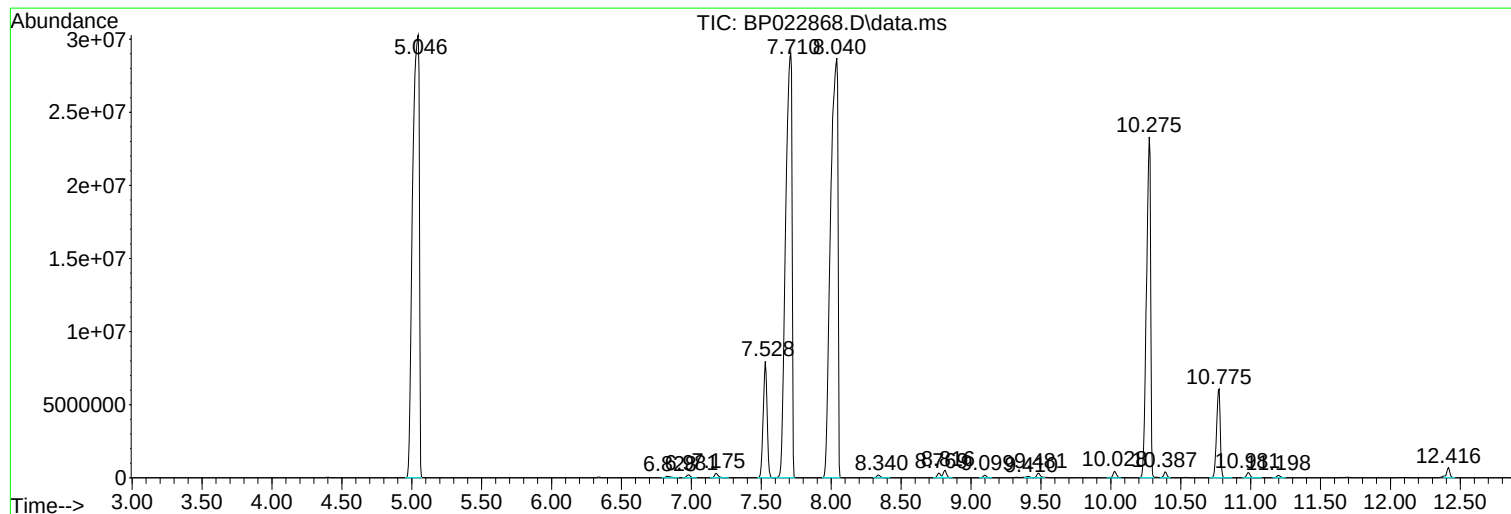
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

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



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Operator : RC/JU
Sample : P4670-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0SY5

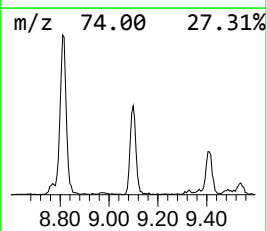
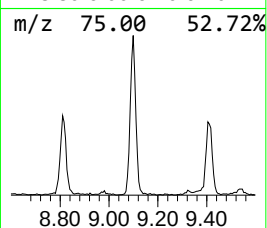
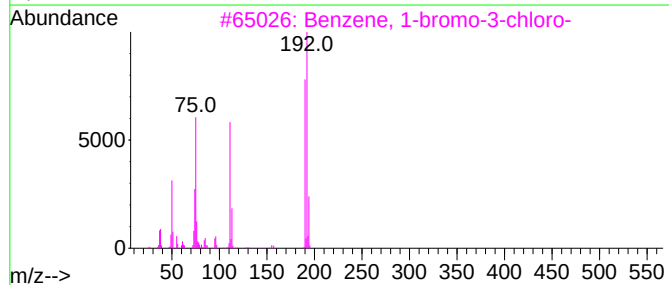
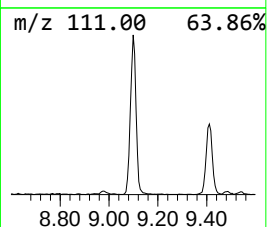
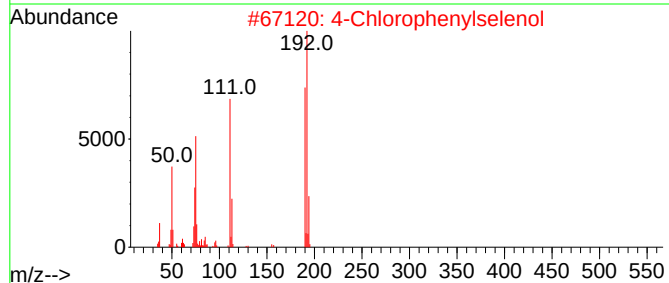
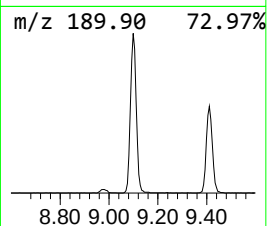
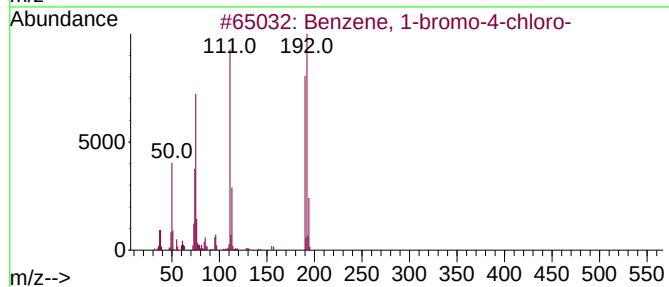
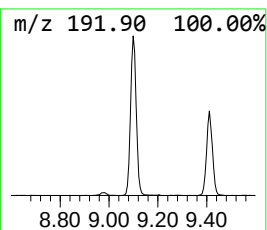
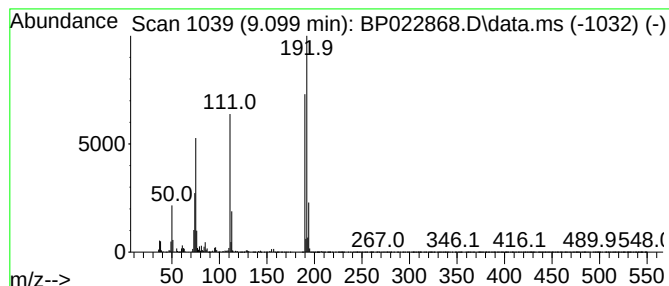
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Benzene, 1-bromo-4-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.099	9.66 ng/ul	292668	Naphthalene-d8	10.387

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
2			4-Chlorophenylselenol	192	C6H5ClSe	016645-10-6	95
3			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	95
4			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	94
5			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	93



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Sample : P4670-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0SY5

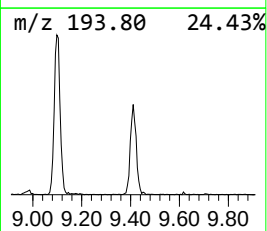
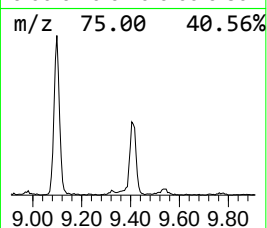
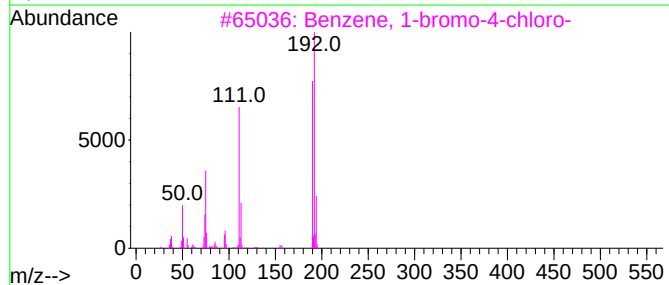
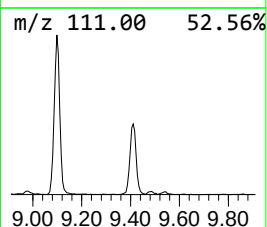
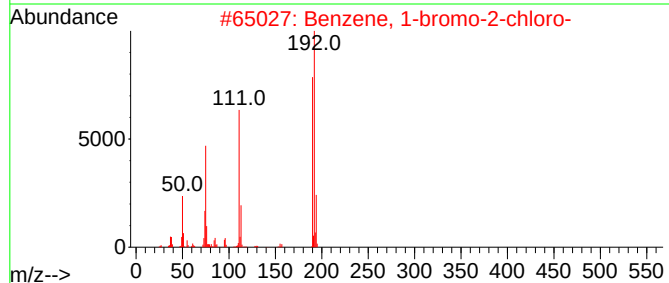
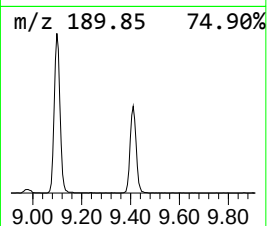
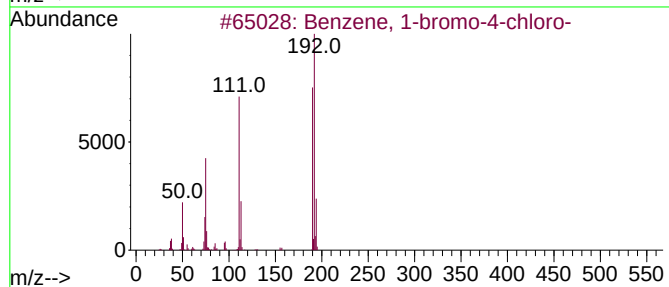
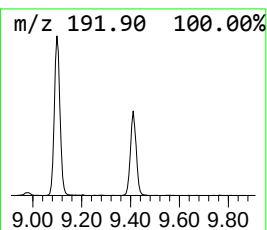
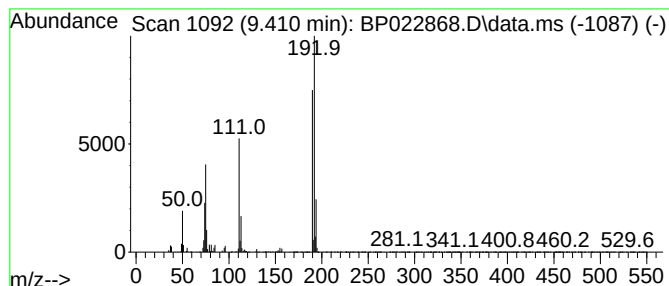
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 Benzene, 1-bromo-2-chloro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	5.51 ng/ul	166850	Naphthalene-d8	10.387

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
2			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
3			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	95
4			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	94
5			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110424\
Data File : BP022868.D
Acq On : 05 Nov 2024 20:14
Operator : RC/JU
Sample : P4670-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0SY5

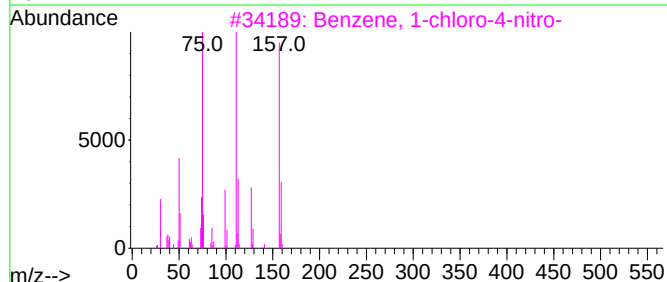
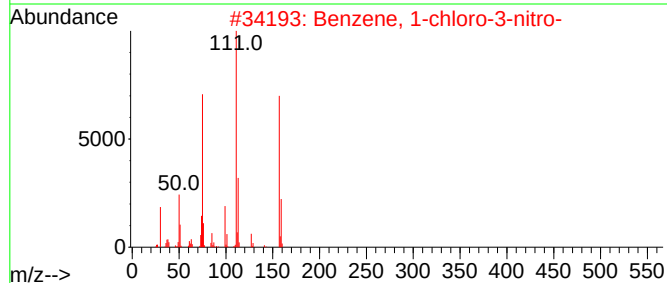
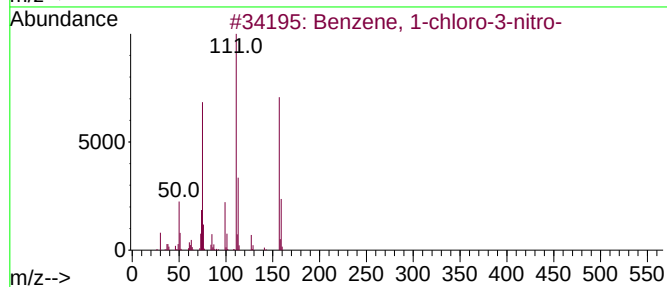
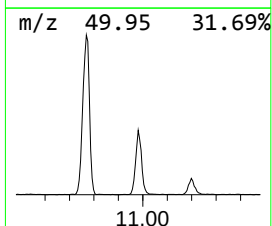
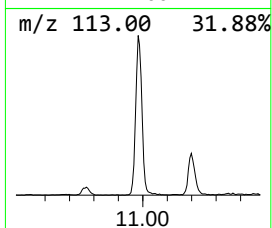
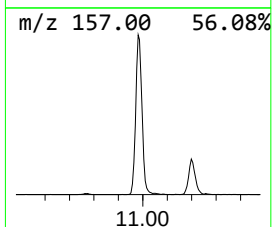
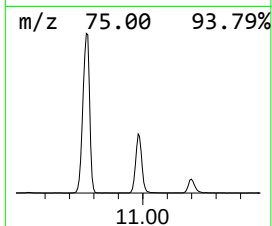
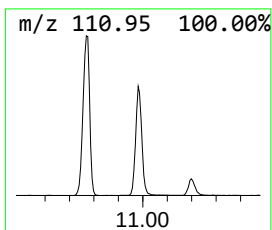
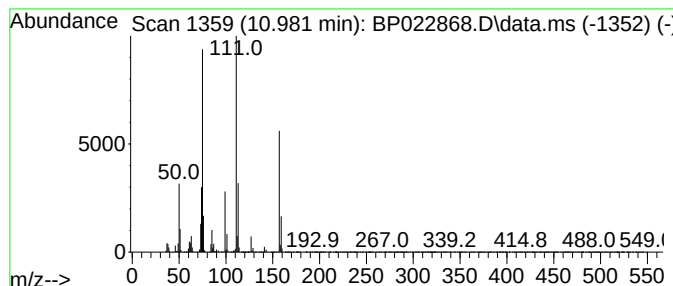
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 9 Benzene, 1-chloro-3-nitro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.981	20.84 ng/ul	631447	Naphthalene-d8	10.387

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-chloro-3-nitro-	157	C6H4ClNO2	000121-73-3	97
2			Benzene, 1-chloro-3-nitro-	157	C6H4ClNO2	000121-73-3	94
3			Benzene, 1-chloro-4-nitro-	157	C6H4ClNO2	000100-00-5	94
4			Benzene, 1-chloro-2-nitro-	157	C6H4ClNO2	000088-73-3	93
5			Benzene, 1-chloro-4-nitro-	157	C6H4ClNO2	000100-00-5	91



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Sample : P4670-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

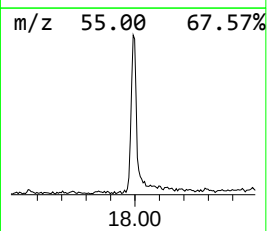
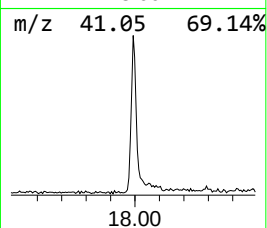
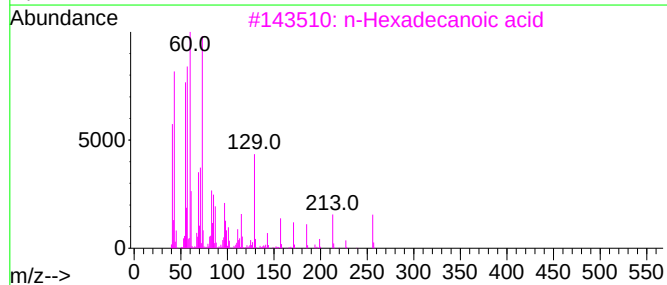
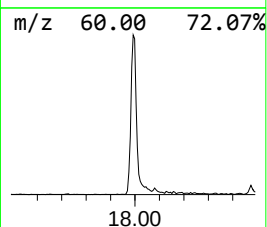
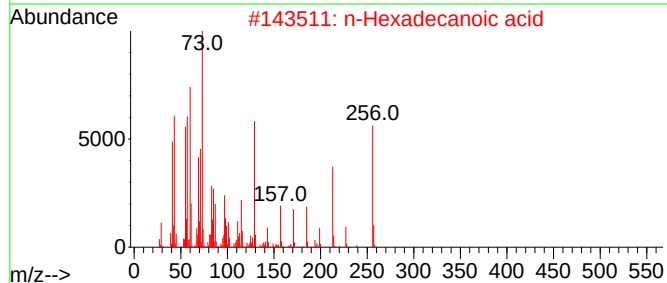
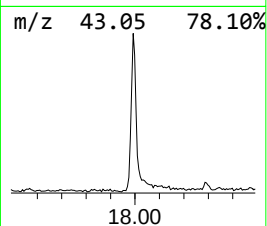
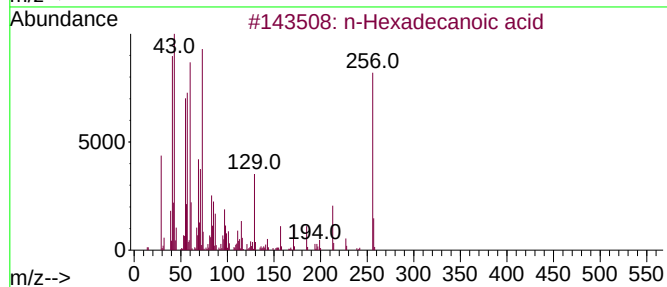
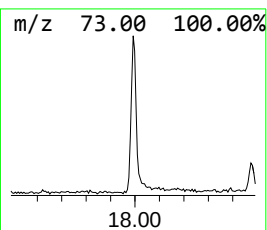
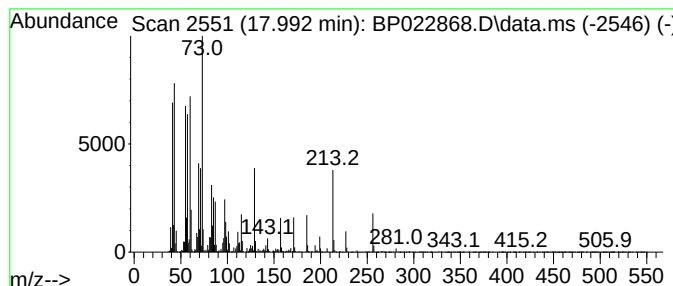
Instrument :
BNA_P
ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 13 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.992	5.55 ng/ul	369831	Phenanthrene-d10	17.051	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
5	Tridecanoic acid	214	C13H26O2	000638-53-9	90



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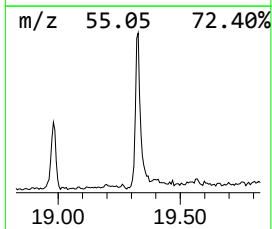
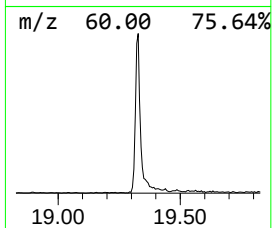
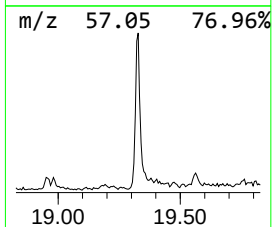
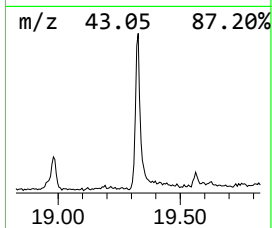
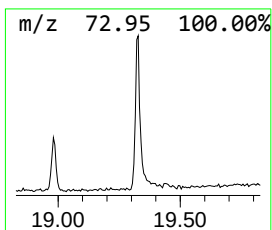
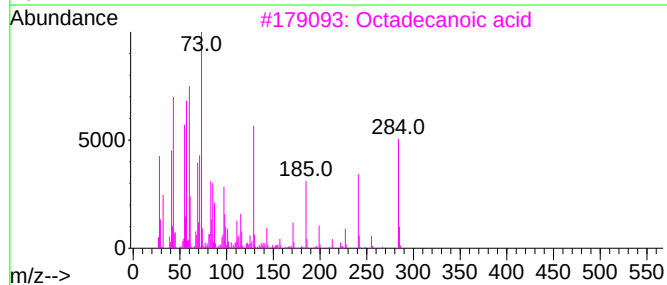
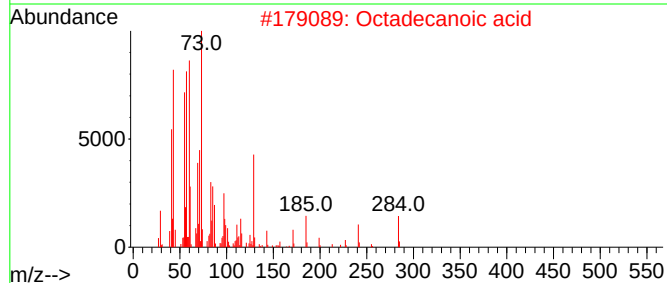
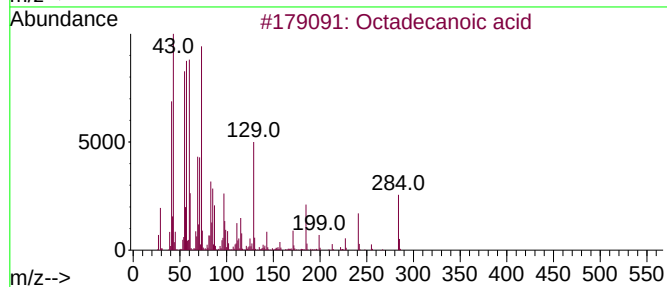
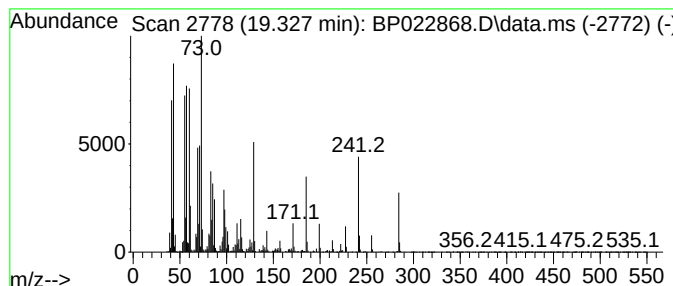
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Quant Title : SVOA CALIBRATION

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

Peak Number 15 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.327	5.77 ng/ul	522774	Chrysene-d12	21.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	95
4			Octadecanoic acid	284	C18H36O2	000057-11-4	93
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110424\
Data File : BP022868.D
Acq On : 05 Nov 2024 20:14
Operator : RC/JU
Sample : P4670-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0SY5

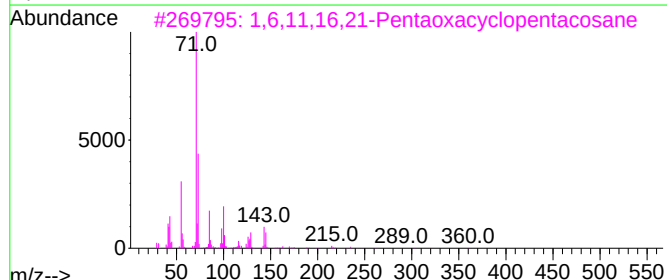
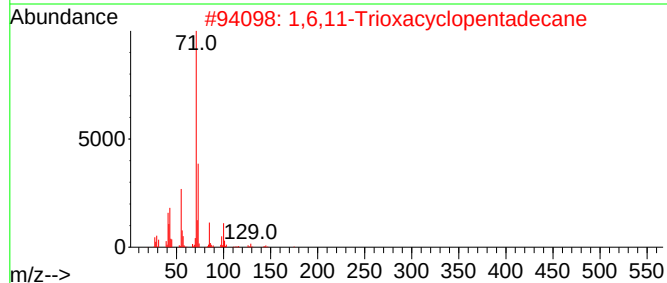
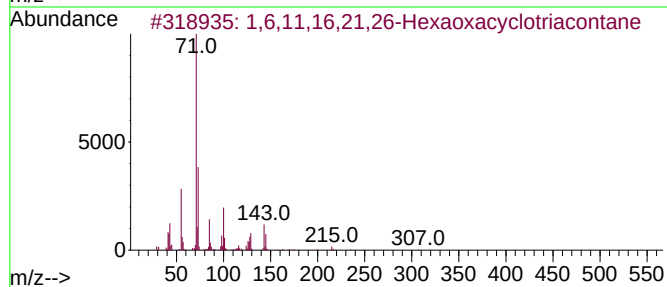
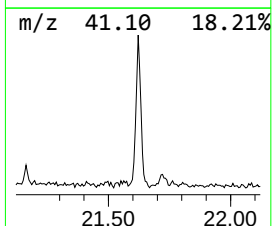
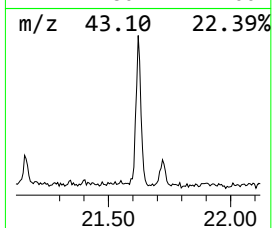
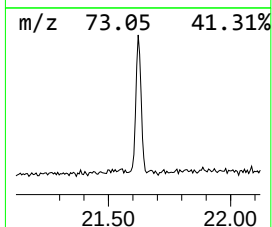
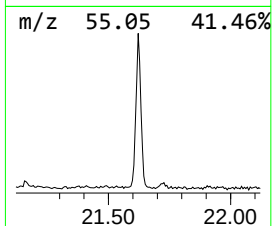
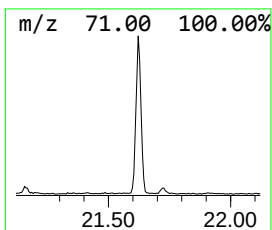
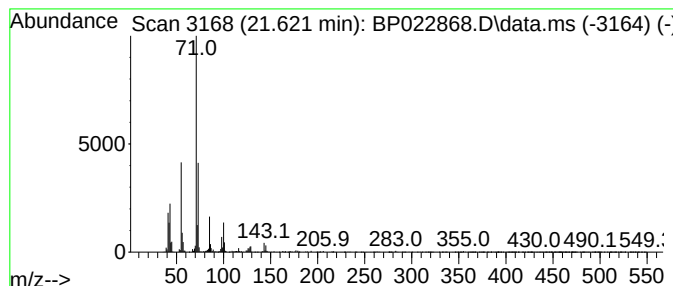
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Quant Title : SVOA CALIBRATION

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

Peak Number 16 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.621	3.95 ng/ul	357839	Chrysene-d12	21.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	91		
2	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	86		
3	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	53		
4	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	50		
5	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110424\
Data File : BP022868.D
Acq On : 05 Nov 2024 20:14
Operator : RC/JU
Sample : P4670-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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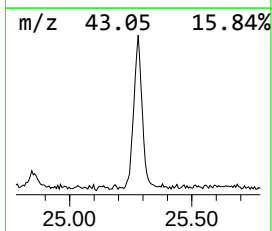
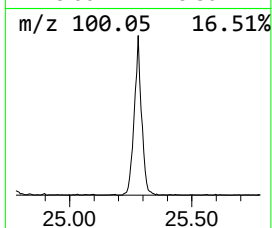
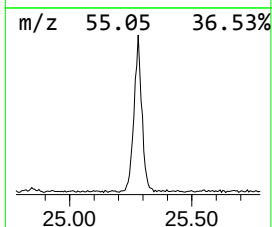
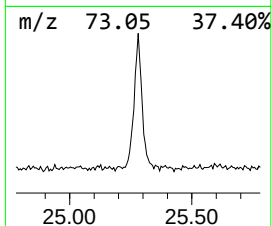
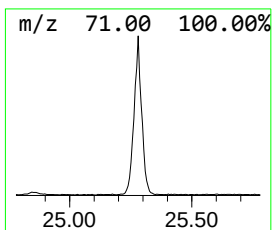
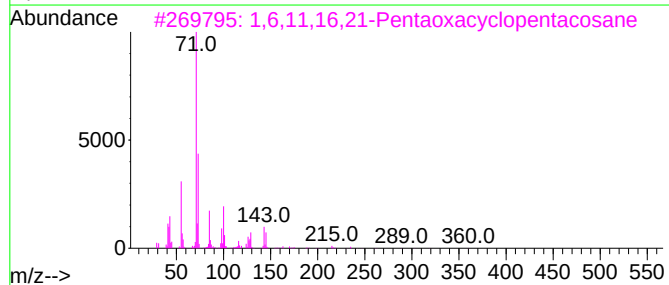
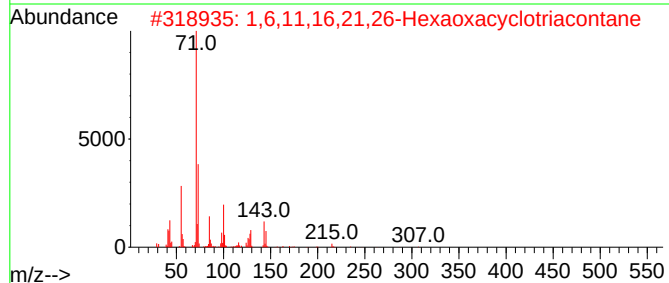
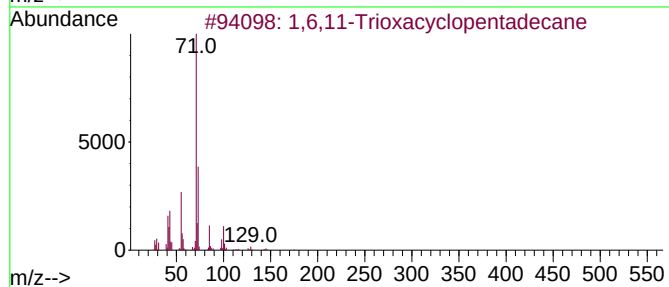
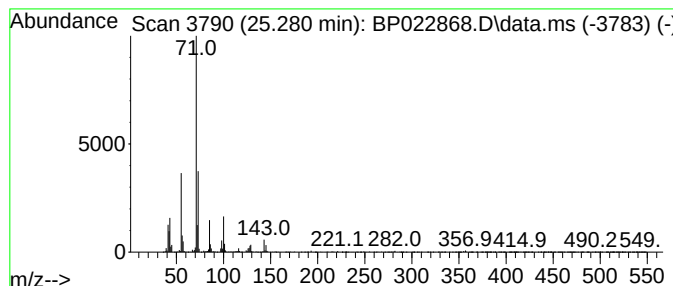
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Quant Title : SVOA CALIBRATION

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

Peak Number 17 1,6,11-Trioxacyclopentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.280	6.02 ng/ul	558862	Perylene-d12	24.751

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	90		
2	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	87		
3	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	58		
4	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	58		
5	./-.-Tetrahydro-3-furanmethanol	102	C5H10O2	015833-61-1	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110424\
Data File : BP022868.D
Acq On : 05 Nov 2024 20:14
Operator : RC/JU
Sample : P4670-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0SY5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP100724.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-brom...	9.099	9.7	ng/ul	292668	2	10.387	605867	20.0
Benzene, 1-brom...	9.410	5.5	ng/ul	166850	2	10.387	605867	20.0
Benzene, 1-chlo...	10.981	20.8	ng/ul	631447	2	10.387	605867	20.0
n-Hexadecanoic ...	17.992	5.5	ng/ul	369831	4	17.051	1333480	20.0
Octadecanoic acid	19.327	5.8	ng/ul	522774	5	21.492	1812350	20.0
1,6,11,16,21,26...	21.621	4.0	ng/ul	357839	5	21.492	1812350	20.0
1,6,11-Trioxacy...	25.280	6.0	ng/ul	558862	6	24.751	1857940	20.0