

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
 Data File : BP018969.D
 Acq On : 20 Dec 2023 20:01
 Operator : MA/JU
 Sample : 05894-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BH3K7

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-BP120123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.675	96	100	116	rVB	184648	282816	0.19%	0.131%
2	6.999	660	665	675	rVB	132761	215486	0.14%	0.100%
3	7.163	687	693	705	rVB	500031	768150	0.51%	0.357%
4	7.357	719	726	736	rVB	485978	756972	0.50%	0.352%
5	7.822	798	805	814	rBV	453589	720556	0.47%	0.335%
6	8.540	920	927	935	rBV	376509	609010	0.40%	0.283%
7	8.987	994	1003	1015	rBV	579782	929929	0.61%	0.432%
8	9.193	1018	1038	1050	rBV	567383	1807287	1.19%	0.840%
9	9.704	1117	1125	1134	rBV	439107	741809	0.49%	0.345%
10	10.246	1207	1217	1231	rBV	680950	1149579	0.76%	0.534%
11	10.616	1274	1280	1289	rVB	546519	929119	0.61%	0.432%
12	10.763	1295	1305	1319	rBV	629028	1062123	0.70%	0.494%
13	13.363	1739	1747	1754	rBV	105458	170686	0.11%	0.079%
14	13.875	1827	1834	1850	rBV	1371253	1864645	1.23%	0.866%
15	14.151	1870	1881	1891	rBV	1520217	2263639	1.49%	1.052%
16	14.269	1895	1901	1910	rVV	179629	280017	0.18%	0.130%
17	14.457	1926	1933	1948	rBV2	832196	1340922	0.88%	0.623%
18	14.687	1965	1972	1981	rBV	86480	179134	0.12%	0.083%
19	15.451	2092	2102	2114	rBV	1991779	3023781	1.99%	1.405%
20	15.581	2117	2124	2136	rBV	578956	816751	0.54%	0.380%
21	17.175	2363	2395	2398	rBV	21940639	151718879	100.00%	70.501%
22	17.216	2399	2402	2412	rVV	1030701	1499620	0.99%	0.697%
23	17.316	2413	2419	2430	rVB	2160307	3023873	1.99%	1.405%
24	18.104	2547	2553	2557	rBV3	136736	244415	0.16%	0.114%
25	18.310	2584	2588	2598	rBV	135700	205537	0.14%	0.096%
26	19.039	2707	2712	2720	rVB	1663143	2065585	1.36%	0.960%
27	19.551	2793	2799	2804	rBV	3260877	4101907	2.70%	1.906%
28	20.633	2981	2983	2987	rVB	318119	361413	0.24%	0.168%
29	20.869	3020	3023	3025	rBV	238421	309119	0.20%	0.144%
30	20.933	3032	3034	3038	rVB	187859	191499	0.13%	0.089%
31	21.304	3092	3097	3105	rBV	1493656	1932597	1.27%	0.898%
32	21.398	3108	3113	3117	rBV	3636425	4452377	2.93%	2.069%
33	22.145	3235	3240	3252	rBV	408638	1087501	0.72%	0.505%
34	23.515	3465	3473	3484	rVB	2475367	5059932	3.34%	2.351%
35	23.663	3492	3498	3508	rVB	1086992	2226071	1.47%	1.034%
36	23.927	3536	3543	3555	rVB	3827221	7801985	5.14%	3.625%

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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-BP120123.MA.M
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37	28.509	4310	4322	4339	rVB	2255954	9006546	5.94%	4.185%
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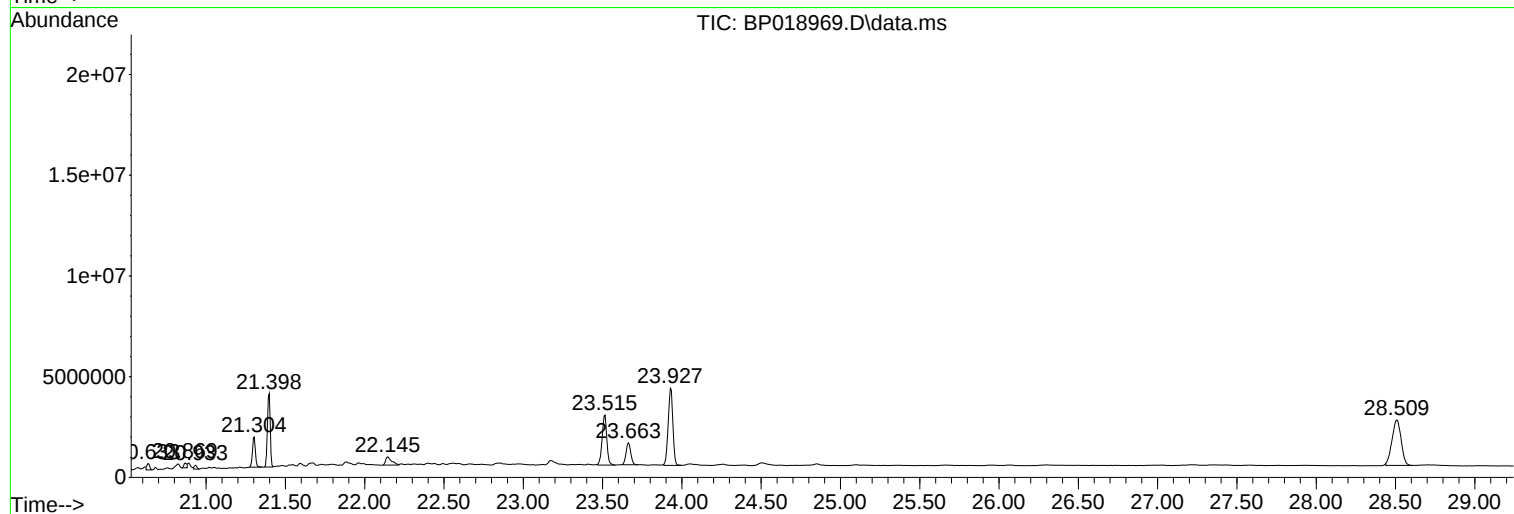
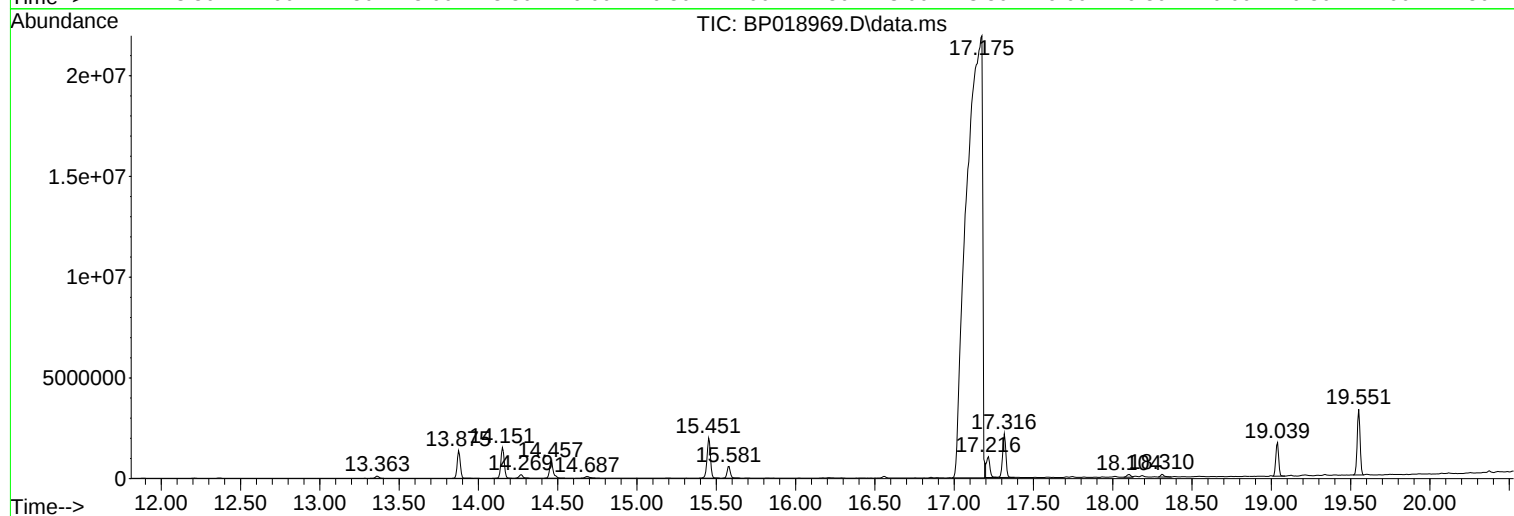
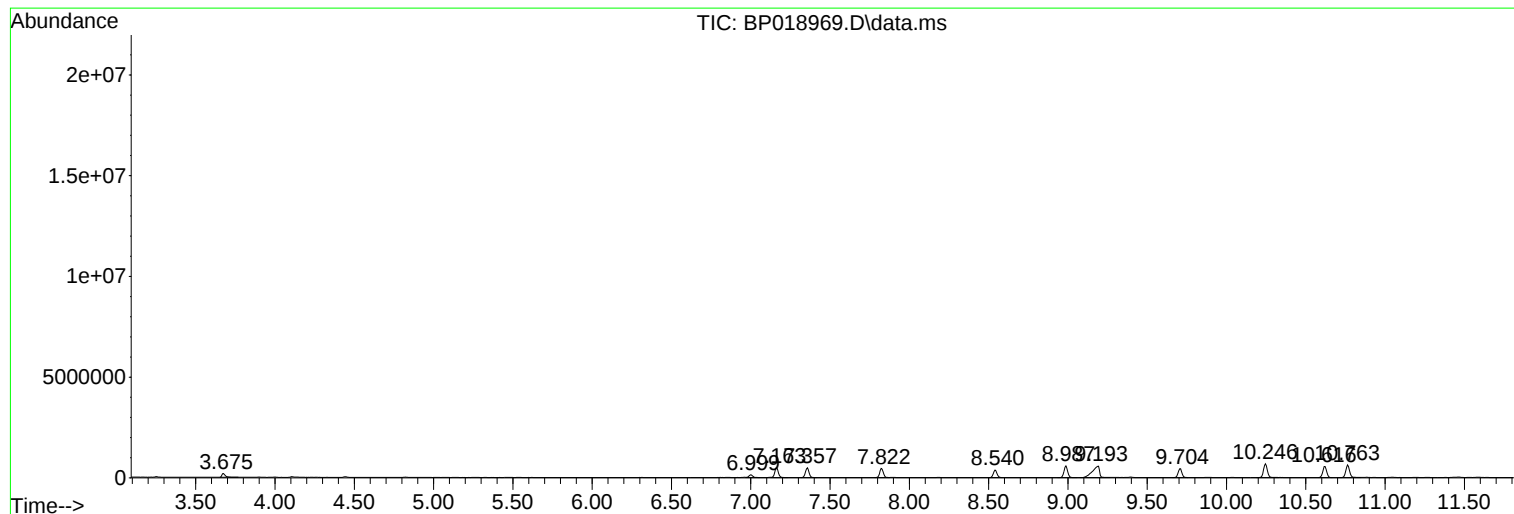
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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



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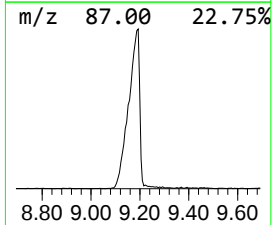
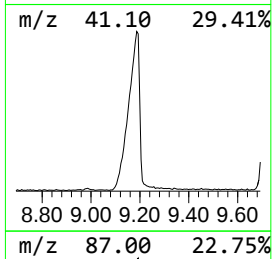
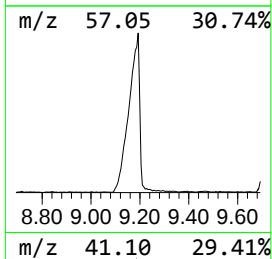
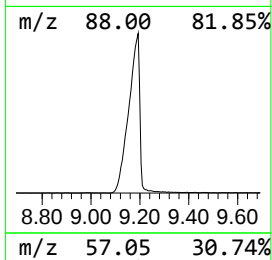
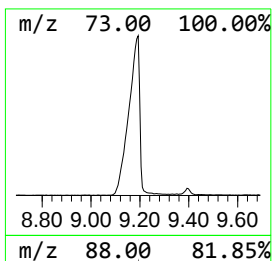
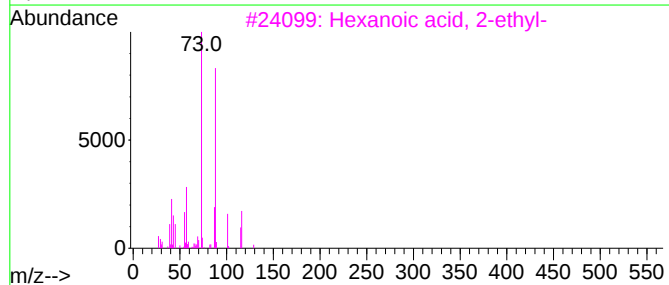
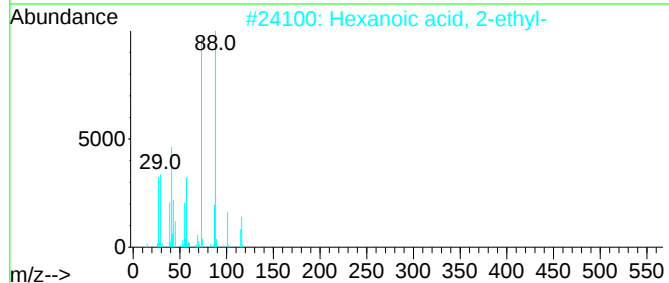
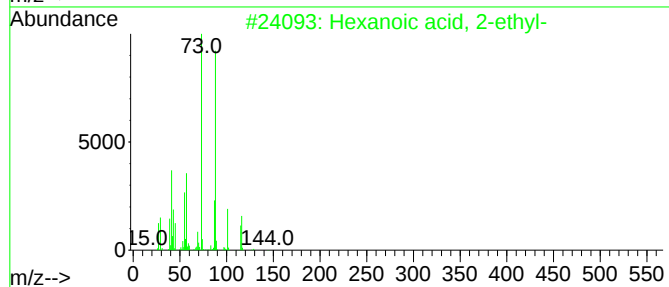
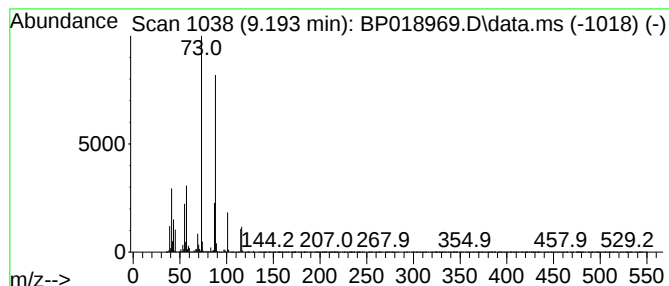
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.193	50.16 ng/ul	1807290	1,4-Dichlorobenzene-d4	7.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
3			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
4			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
5			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72



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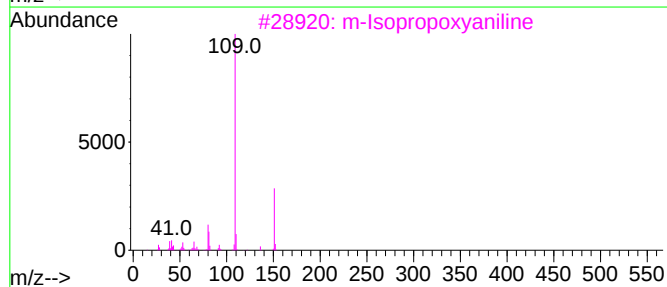
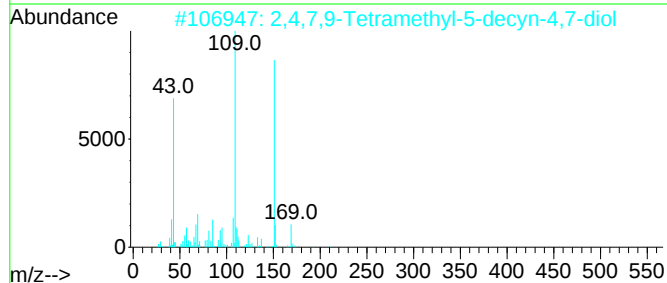
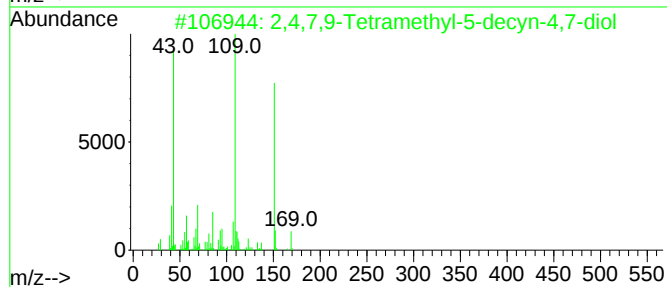
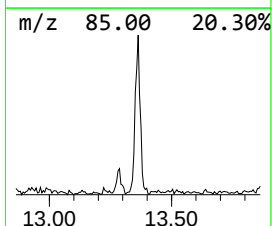
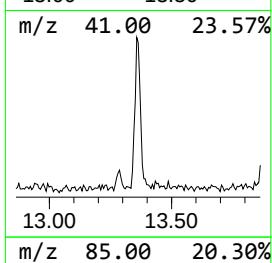
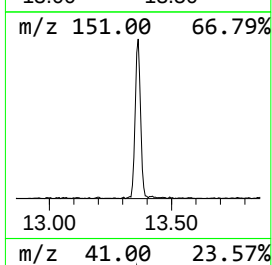
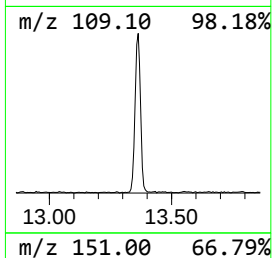
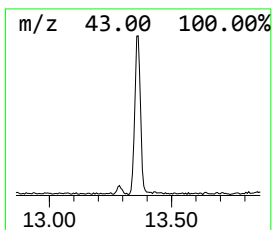
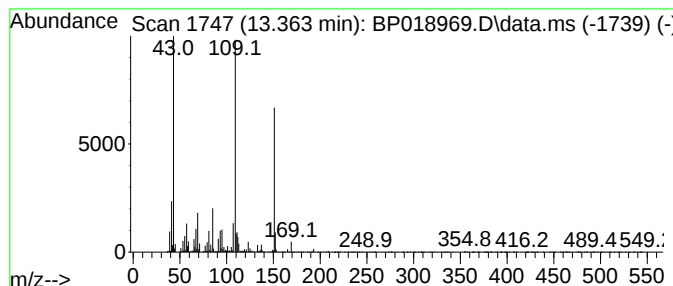
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TIC Library : C:\DATABASE\NIST20.L
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Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.363	2.55 ng/ul	170686	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87		
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50		
4	Metacetamol	151	C8H9NO2	000621-42-1	50		
5	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43		



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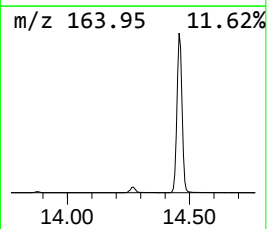
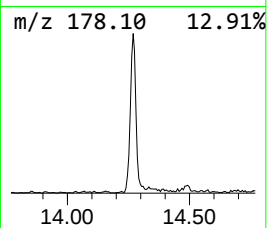
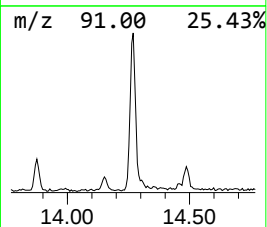
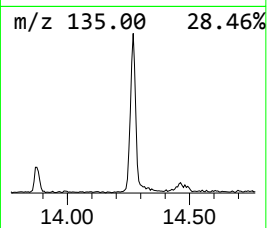
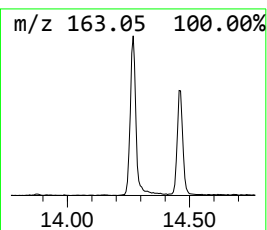
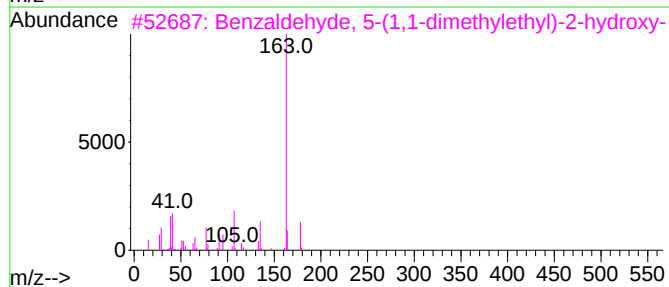
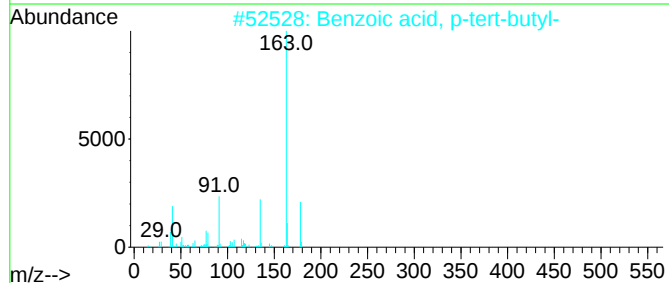
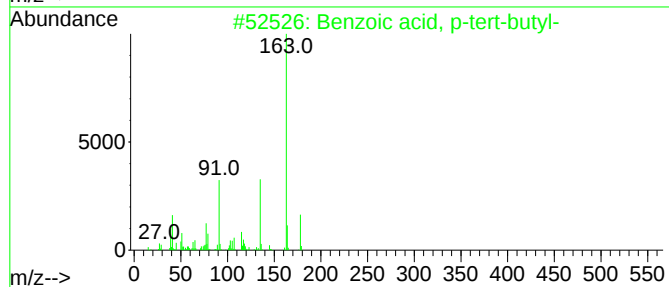
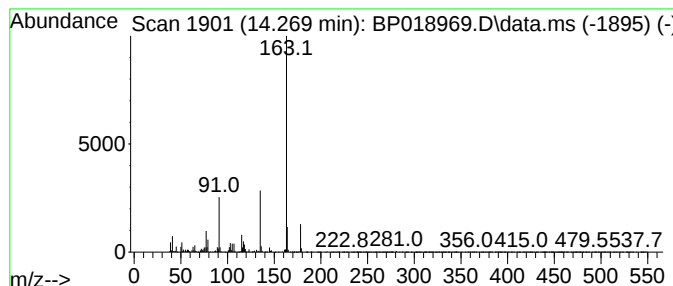
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzoic acid, p-tert-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	4.18 ng/ul	280017	Acenaphthene-d10	14.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	90
3			Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	72
4			Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
5			1,3-Benzenedicarboxylic acid, di...	194	C10H10O4	001459-93-4	64



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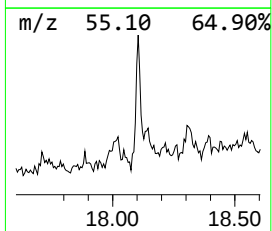
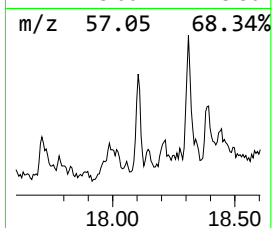
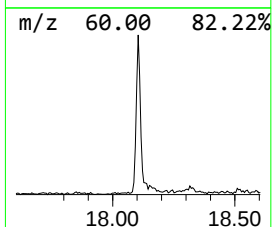
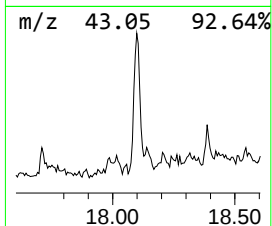
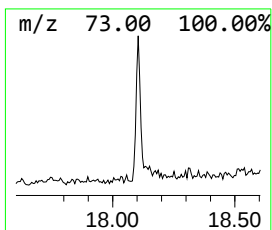
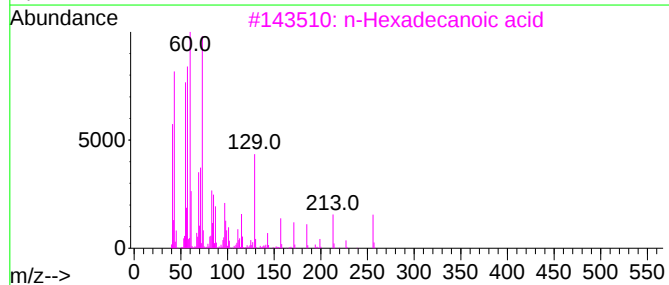
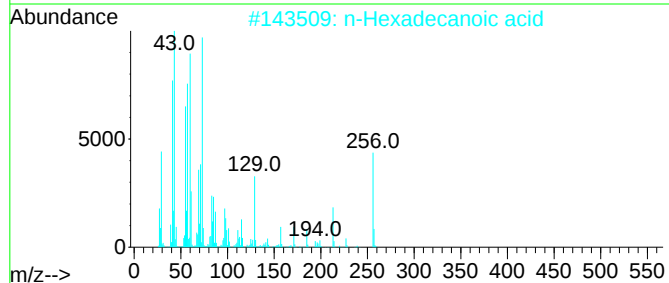
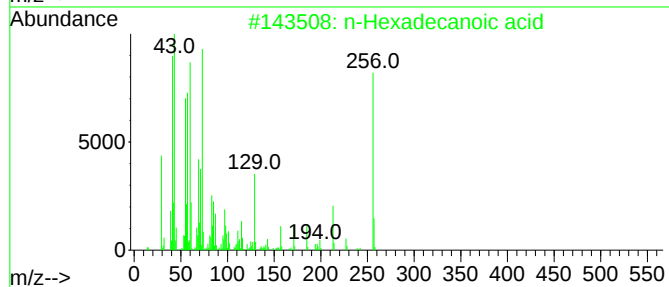
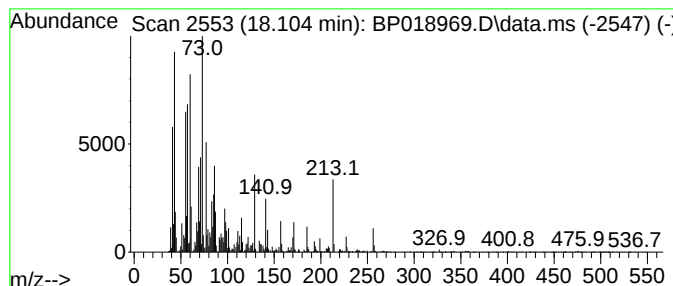
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.104	3.26 ng/ul	244415	Phenanthrene-d10	17.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	92
5			Tridecanoic acid	214	C13H26O2	000638-53-9	90



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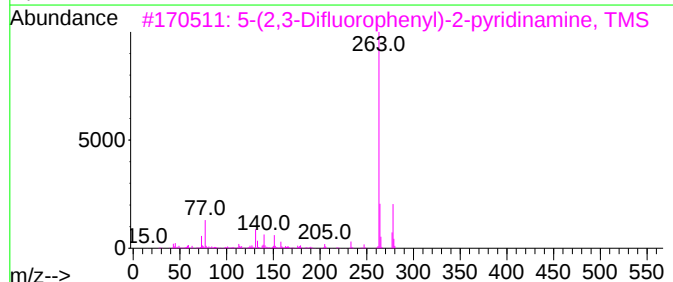
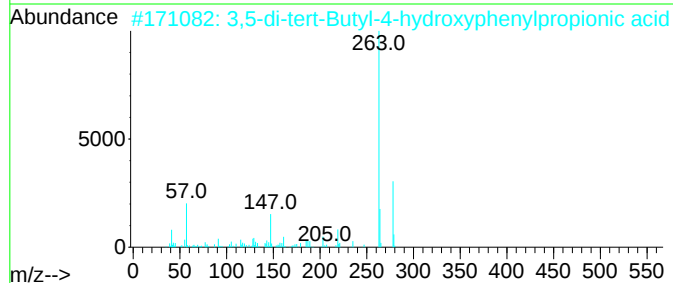
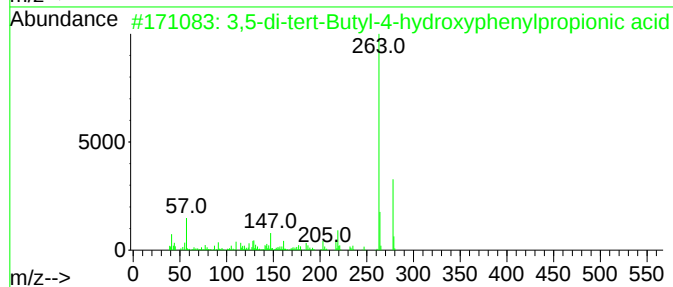
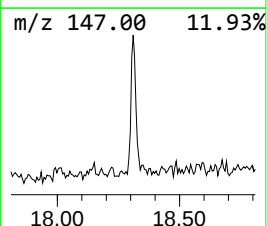
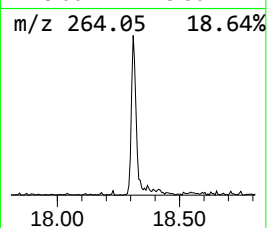
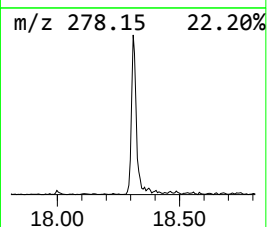
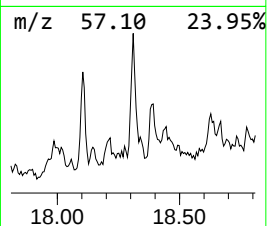
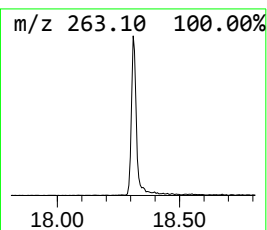
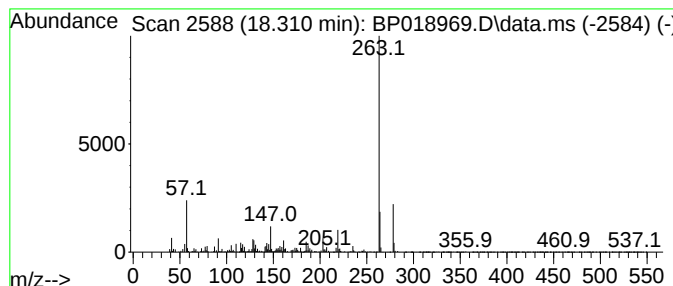
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.310	2.74 ng/ul	205537	Phenanthrene-d10	17.216	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	93
2	3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	92
3	5-(2,3-Difluorophenyl)-2-pyridin...	278	C14H16F2N2Si	1000504-49-4	81
4	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	64
5	Cyanic acid, (1-methylethylidene...	278	C17H14N2O2	001156-51-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
Data File : BP018969.D
Acq On : 20 Dec 2023 20:01
Operator : MA/JU
Sample : 05894-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

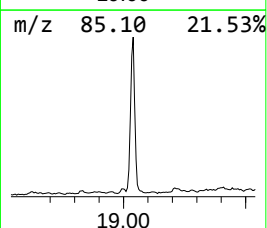
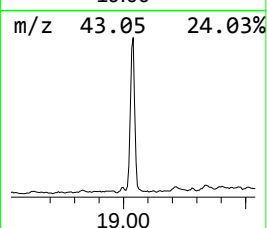
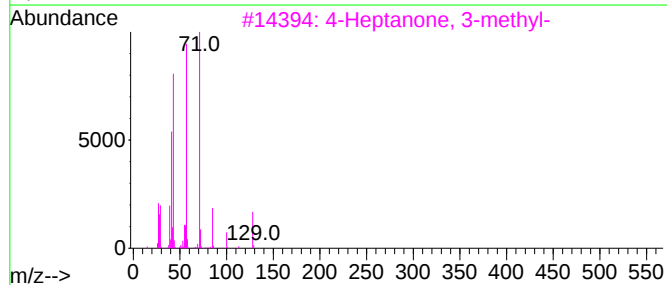
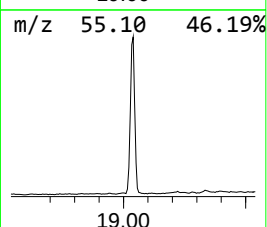
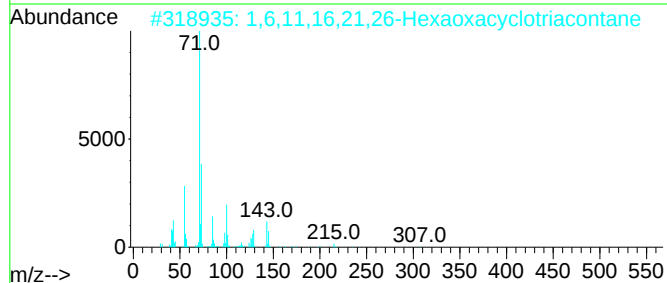
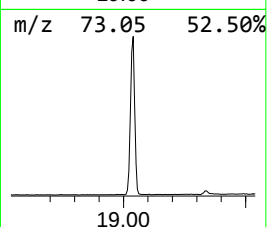
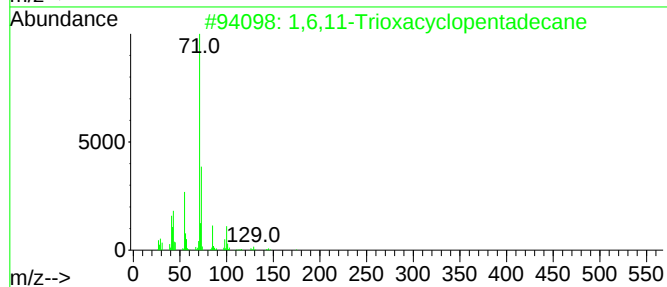
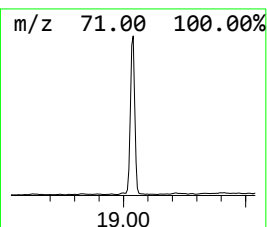
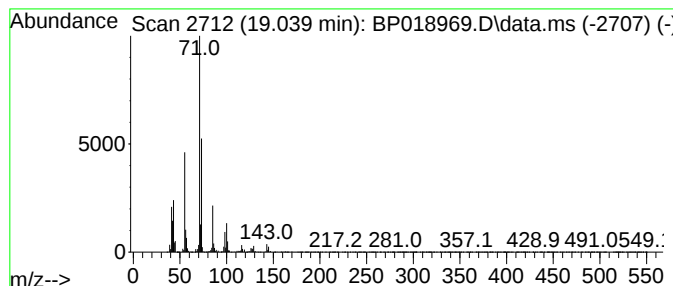
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 1,6,11-Trioxacyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
19.039	27.55 ng/ul	2065590	Phenanthrene-d10			17.216
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,6,11-Trioxacyclopentadecane		216	C12H24O3	000295-63-6	86
2	1,6,11,16,21,26-Hexaoxacyclotria...		432	C24H48O6	064001-05-4	78
3	4-Heptanone, 3-methyl-		128	C8H16O	015726-15-5	64
4	1-Penten-3-ol, 2-methyl-		100	C6H12O	002088-07-5	64
5	1,6,11,16-Tetraoxacycloeicosane		288	C16H32O4	017043-02-6	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
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Sample : 05894-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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ClientSampleId :
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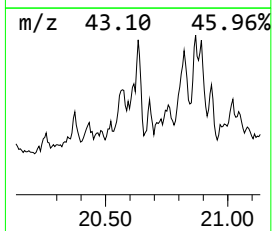
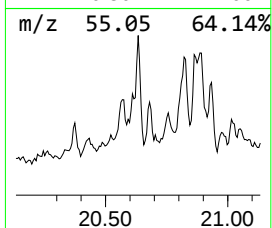
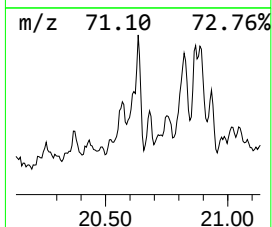
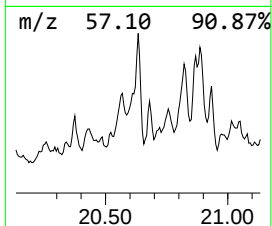
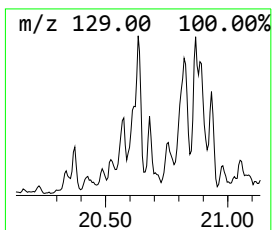
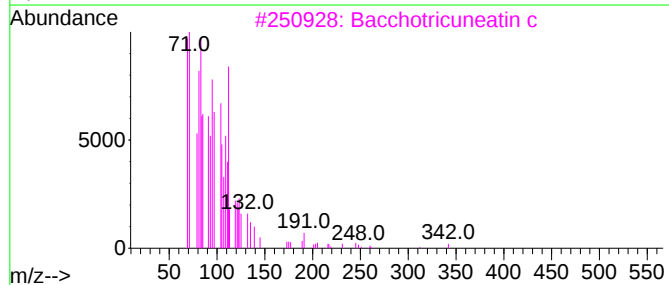
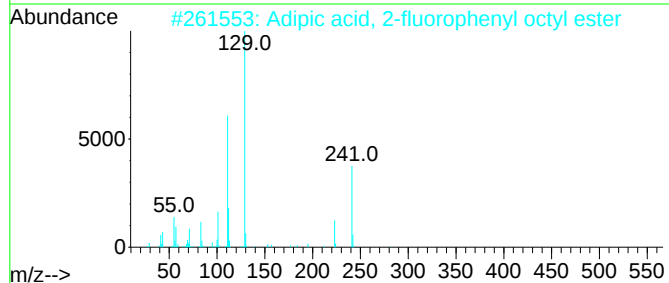
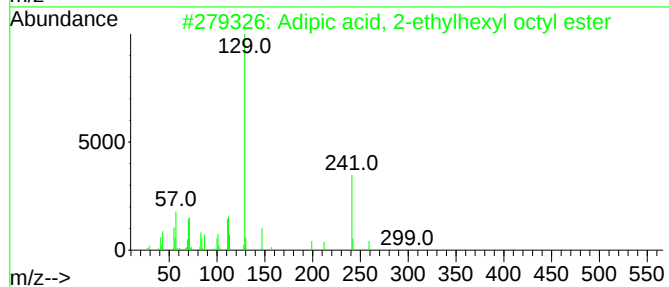
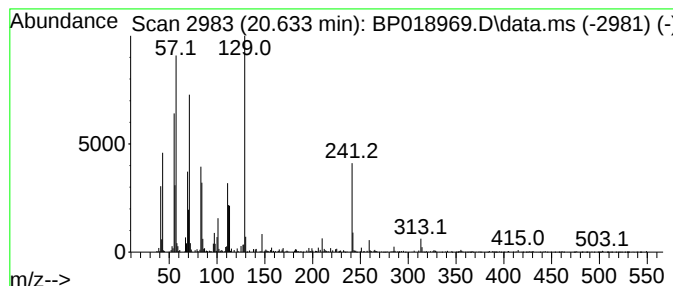
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.633	3.74 ng/ul	361413	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	43
2			Adipic acid, 2-fluorophenyl octy...	352	C20H29FO4	1010324-79-7	43
3			Bacchotricuneatin c	342	C20H22O5	066563-30-2	38
4			2-Heptenoic acid, nonyl ester	254	C16H30O2	1000406-09-5	30
5			Adipic acid, di(but-2-en-1-yl) e...	254	C14H22O4	1000324-71-1	30



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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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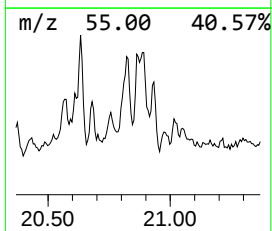
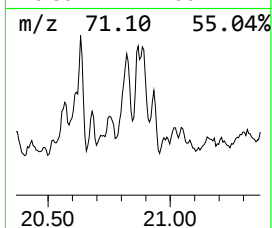
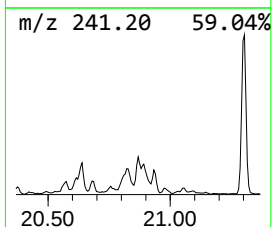
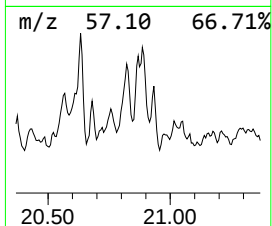
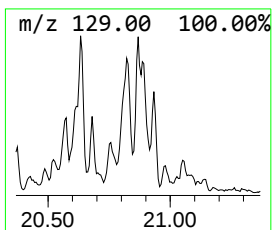
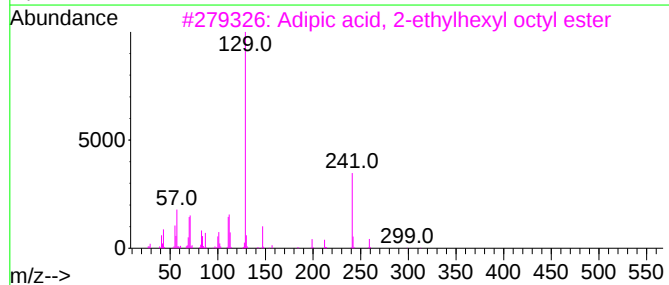
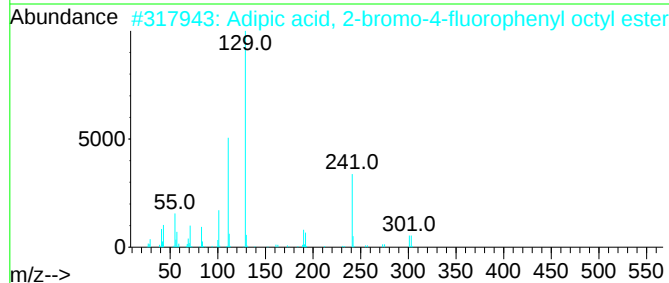
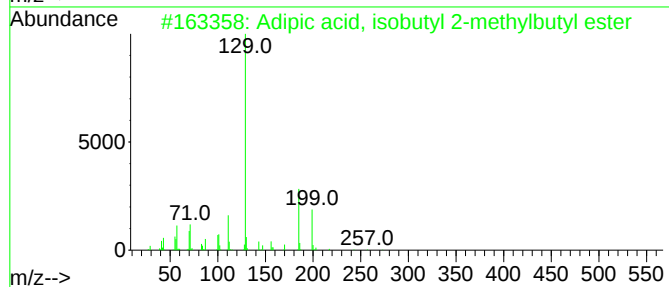
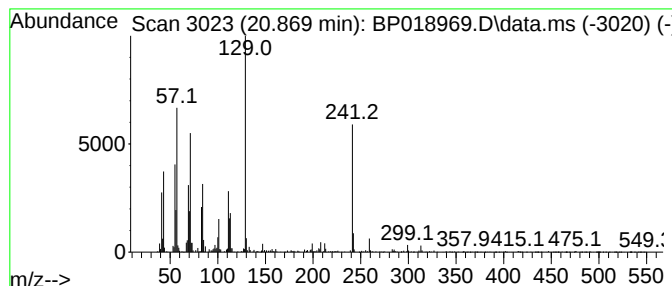
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 Adipic acid, isobutyl 2-met... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.869	3.20 ng/ul	309119	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Adipic acid, isobutyl 2-methylbu...	272	C15H28O4	1000324-67-1	50
2			Adipic acid, 2-bromo-4-fluorophe...	430	C20H28BrFO4	1000324-50-3	50
3			Adipic acid, 2-ethylhexyl octyl ...	370	C22H42O4	1000324-48-6	50
4			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	47
5			Adipic acid, octyl 2,3,6-trichlo...	436	C20H27Cl3O4	1000353-93-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
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Misc :
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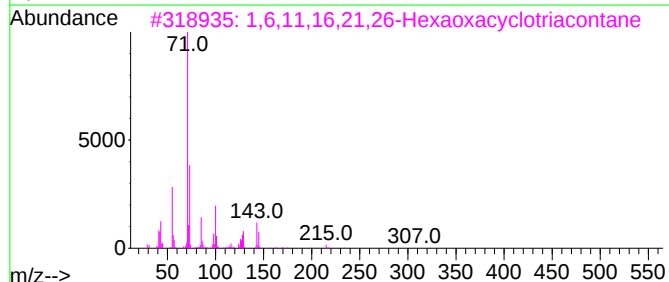
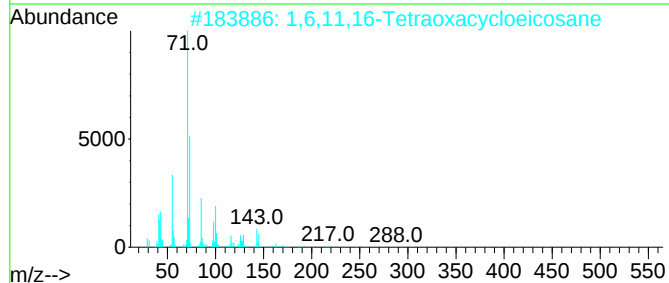
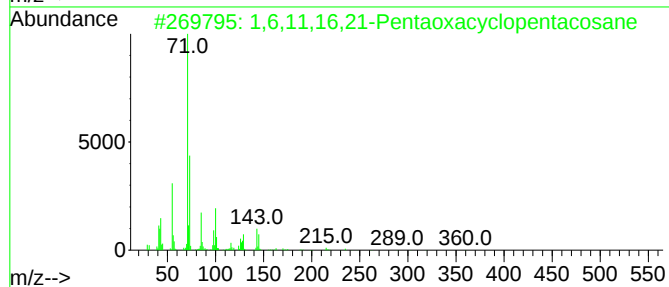
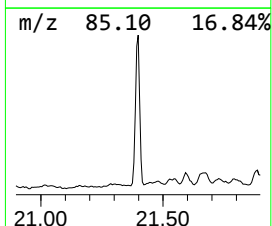
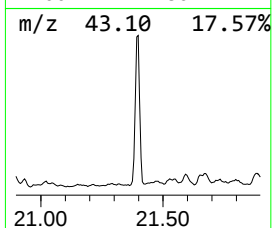
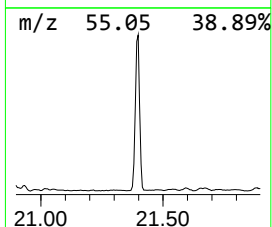
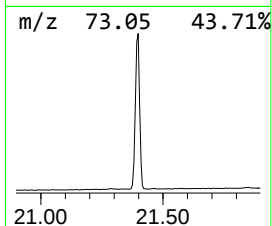
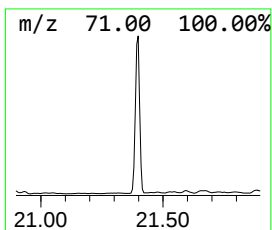
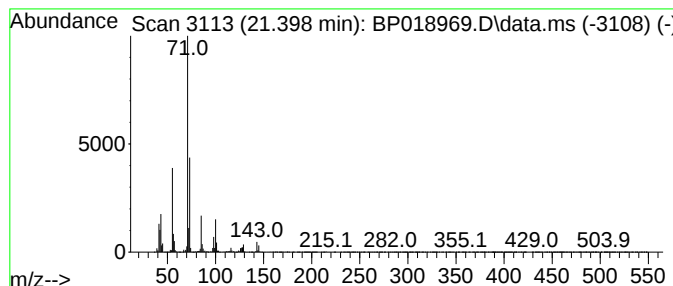
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 1,6,11,16,21-Pentaoxacyclo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.398	46.08 ng/ul	4452380	Chrysene-d12	21.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	91		
2	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	90		
3	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	90		
4	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	64		
5	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	53		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
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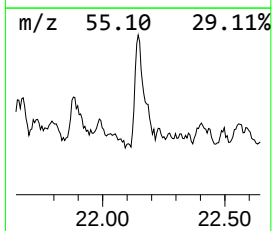
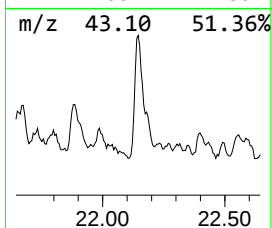
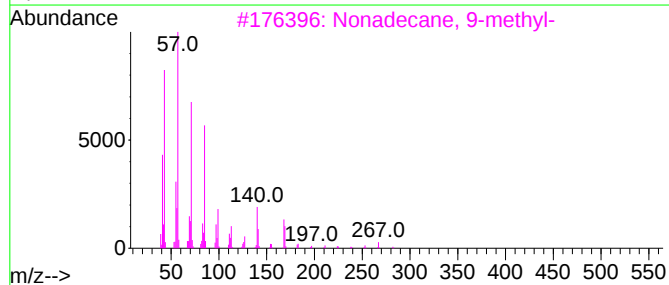
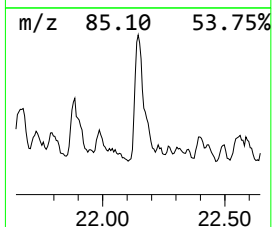
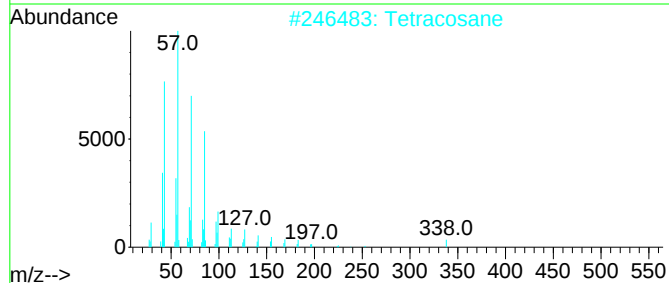
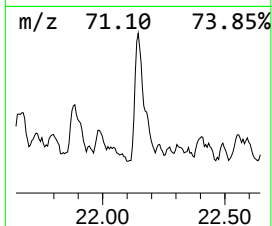
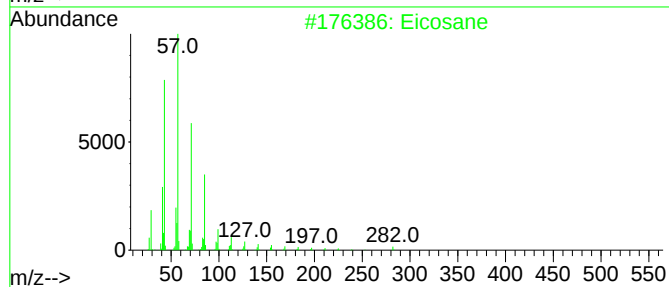
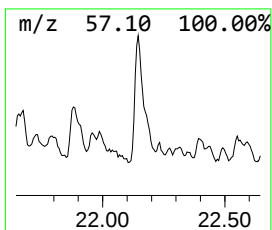
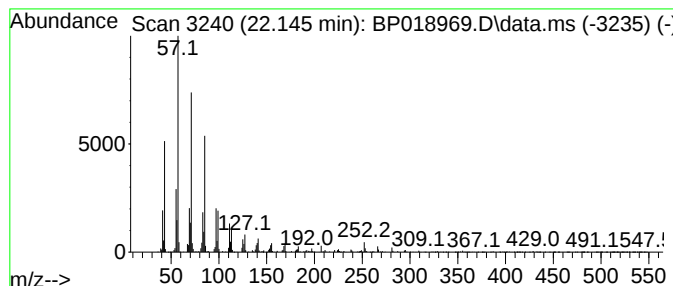
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.145	11.25 ng/ul	1087500	Chrysene-d12	21.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	95
2		Tetracosane	338	C24H50	000646-31-1	93
3		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
4		Heptadecane	240	C17H36	000629-78-7	91
5		Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
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Misc :
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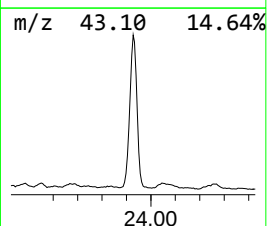
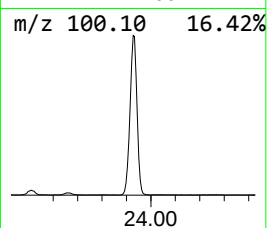
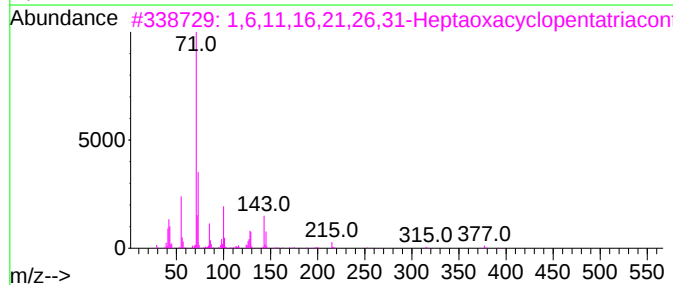
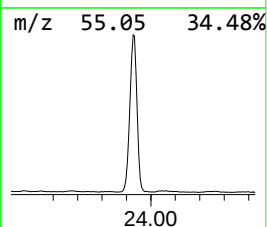
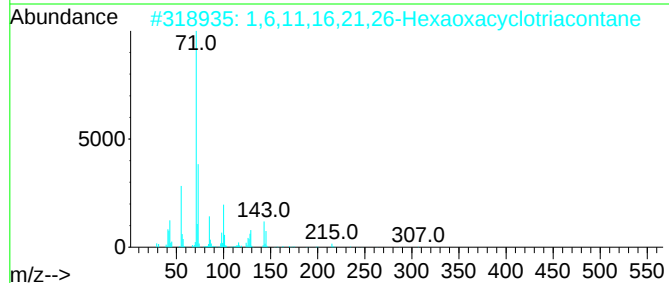
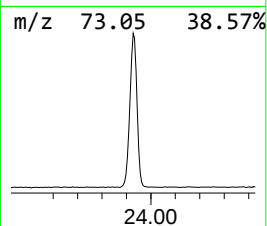
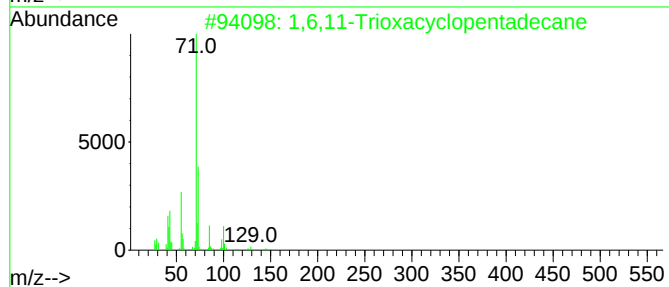
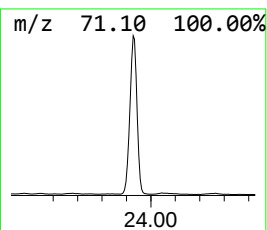
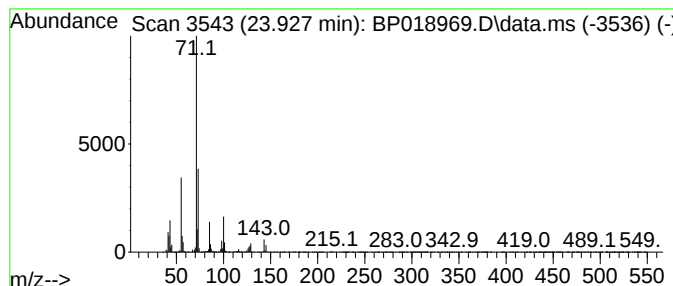
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.927	70.10 ng/ul	7801990	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11	-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	86	
2	1,6,11,16,21,26	-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	74	
3	1,6,11,16,21,26,31	-Heptaoxacyclo...	504	C28H56O7	066055-34-3	59	
4	Acrolein,dimethyl	acetal	102	C5H10O2	006044-68-4	50	
5	./+/-	-Tetrahydro-3-furanmethanol	102	C5H10O2	015833-61-1	47	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
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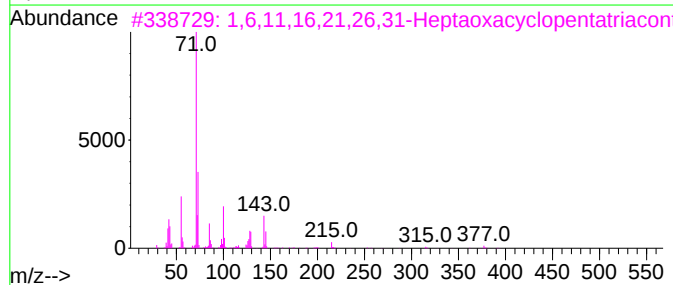
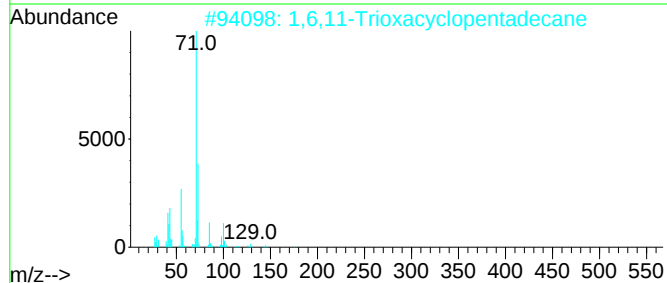
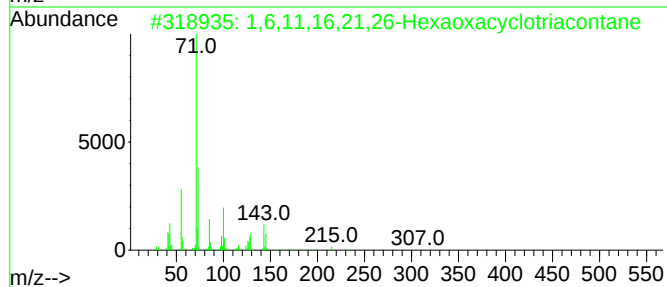
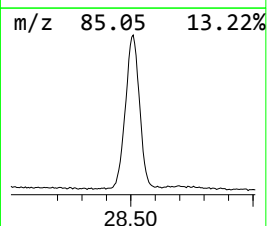
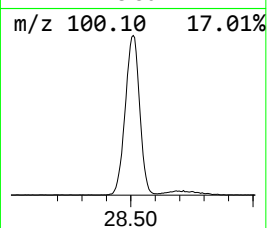
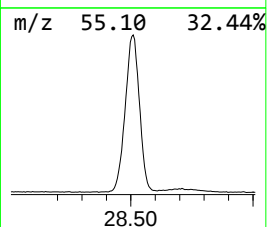
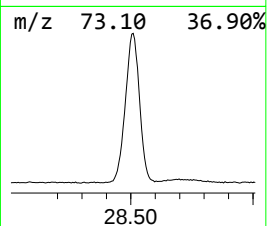
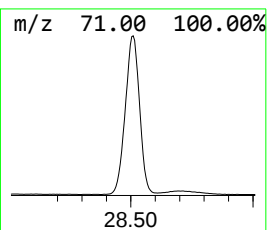
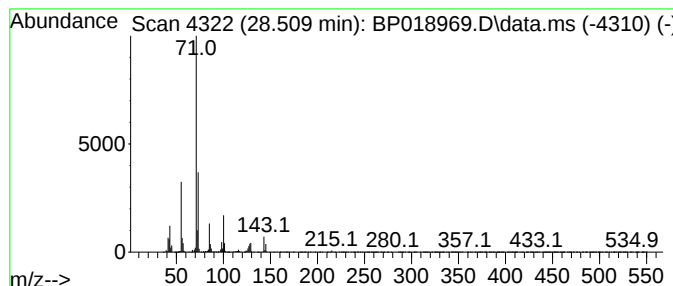
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 12 1,6,11,16,21,26,31-Heptaoxa... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.509	80.92 ng/ul	9006550	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	90		
2	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	80		
3	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	52		
4	.+/-.-Tetrahydro-3-furanmethanol	102	C5H10O2	015833-61-1	47		
5	Acrolein,dimethyl acetal	102	C5H10O2	006044-68-4	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122023\
Data File : BP018969.D
Acq On : 20 Dec 2023 20:01
Operator : MA/JU
Sample : 05894-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BH3K7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.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
Hexanoic acid, ...	9.193	50.2	ng/ul	1807290	1	7.822	720556	20.0
2,4,7,9-Tetrame...	13.363	2.5	ng/ul	170686	3	14.457	1340920	20.0
Benzoic acid, p...	14.269	4.2	ng/ul	280017	3	14.457	1340920	20.0
n-Hexadecanoic ...	18.104	3.3	ng/ul	244415	4	17.216	1499620	20.0
3,5-di-tert-But...	18.310	2.7	ng/ul	205537	4	17.216	1499620	20.0
1,6,11-Trioxacy...	19.039	27.6	ng/ul	2065590	4	17.216	1499620	20.0
unknown-01	20.633	3.7	ng/ul	361413	5	21.304	1932600	20.0
Adipic acid, is...	20.869	3.2	ng/ul	309119	5	21.304	1932600	20.0
1,6,11,16,21-Pe...	21.398	46.1	ng/ul	4452380	5	21.304	1932600	20.0
(DEL) Alkane: S...	22.145	11.3	ng/ul	1087500	5	21.304	1932600	20.0
1,6,11,16,21,26...	23.927	70.1	ng/ul	7801990	6	23.663	2226070	20.0
1,6,11,16,21,26...	28.509	80.9	ng/ul	9006550	6	23.663	2226070	20.0