

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
 Data File : BM043538.D
 Acq On : 22 Dec 2023 14:07
 Operator : MA/JU
 Sample : 05927-05
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BGWA5

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_M\Methods\SFAM-EPA-BM121523.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BM043538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.799	100	104	119	rBV	347264	611133	0.22%	0.137%
2	4.563	229	234	245	rVB	292157	403147	0.14%	0.090%
3	7.128	663	670	679	rBV	350198	579786	0.21%	0.130%
4	7.304	693	700	711	rBV	1161032	1835974	0.65%	0.410%
5	7.492	726	732	742	rBV	1135242	1796060	0.64%	0.401%
6	7.969	805	813	820	rBV	803526	1293086	0.46%	0.289%
7	8.675	925	933	942	rBV	934169	1493344	0.53%	0.334%
8	9.139	1004	1012	1023	rBV	1367527	2220898	0.79%	0.496%
9	9.863	1127	1135	1143	rBV	949919	1625086	0.58%	0.363%
10	10.392	1218	1225	1238	rBV	1418563	2401596	0.85%	0.537%
11	10.775	1281	1290	1298	rBV	1077541	1835533	0.65%	0.410%
12	10.922	1305	1315	1328	rBV	1272705	2280638	0.81%	0.510%
13	13.504	1747	1754	1762	rBV	387200	628489	0.22%	0.140%
14	14.021	1832	1842	1851	rBV	2510248	3596099	1.28%	0.804%
15	14.298	1877	1889	1901	rBV2	2911344	4359601	1.55%	0.975%
16	14.604	1934	1941	1951	rBV	1480684	2250104	0.80%	0.503%
17	14.810	1970	1976	1997	rBV	193323	388559	0.14%	0.087%
18	15.598	2099	2110	2118	rBV	3769411	5674420	2.02%	1.268%
19	15.715	2124	2130	2144	rBV	1040780	1434221	0.51%	0.321%
20	16.362	2233	2240	2248	rBV	156323	304779	0.11%	0.068%
21	16.704	2293	2298	2313	rBV	163949	376967	0.13%	0.084%
22	17.286	2369	2397	2398	rBV4	48365918	281149395	100.00%	62.847%
23	17.457	2420	2426	2445	rVB	3937554	5567066	1.98%	1.244%
24	18.168	2541	2547	2554	rVV3	288453	497399	0.18%	0.111%
25	18.251	2556	2561	2566	rVV	456889	731242	0.26%	0.163%
26	18.298	2566	2569	2572	rVV	251953	370813	0.13%	0.083%
27	18.345	2573	2577	2583	rVV	231879	397458	0.14%	0.089%
28	19.215	2720	2725	2732	rBV	8489498	10219591	3.63%	2.284%
29	19.739	2808	2814	2821	rVB	4693135	5966785	2.12%	1.334%
30	21.533	3113	3119	3126	rBV	1774952	2342534	0.83%	0.524%
31	21.639	3132	3137	3145	rBV	21739602	26407177	9.39%	5.903%
32	23.791	3495	3503	3515	rBV2	3143463	6009574	2.14%	1.343%
33	23.944	3523	3529	3544	rVB	1176275	2460306	0.88%	0.550%
34	24.262	3573	3583	3605	rBV	21029796	43531511	15.48%	9.731%
35	29.020	4378	4392	4413	rVB	6290623	24314918	8.65%	5.435%

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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_M\Methods\SFAM-EPA-BM121523.MA.M
Title : SVOA CALIBRATION

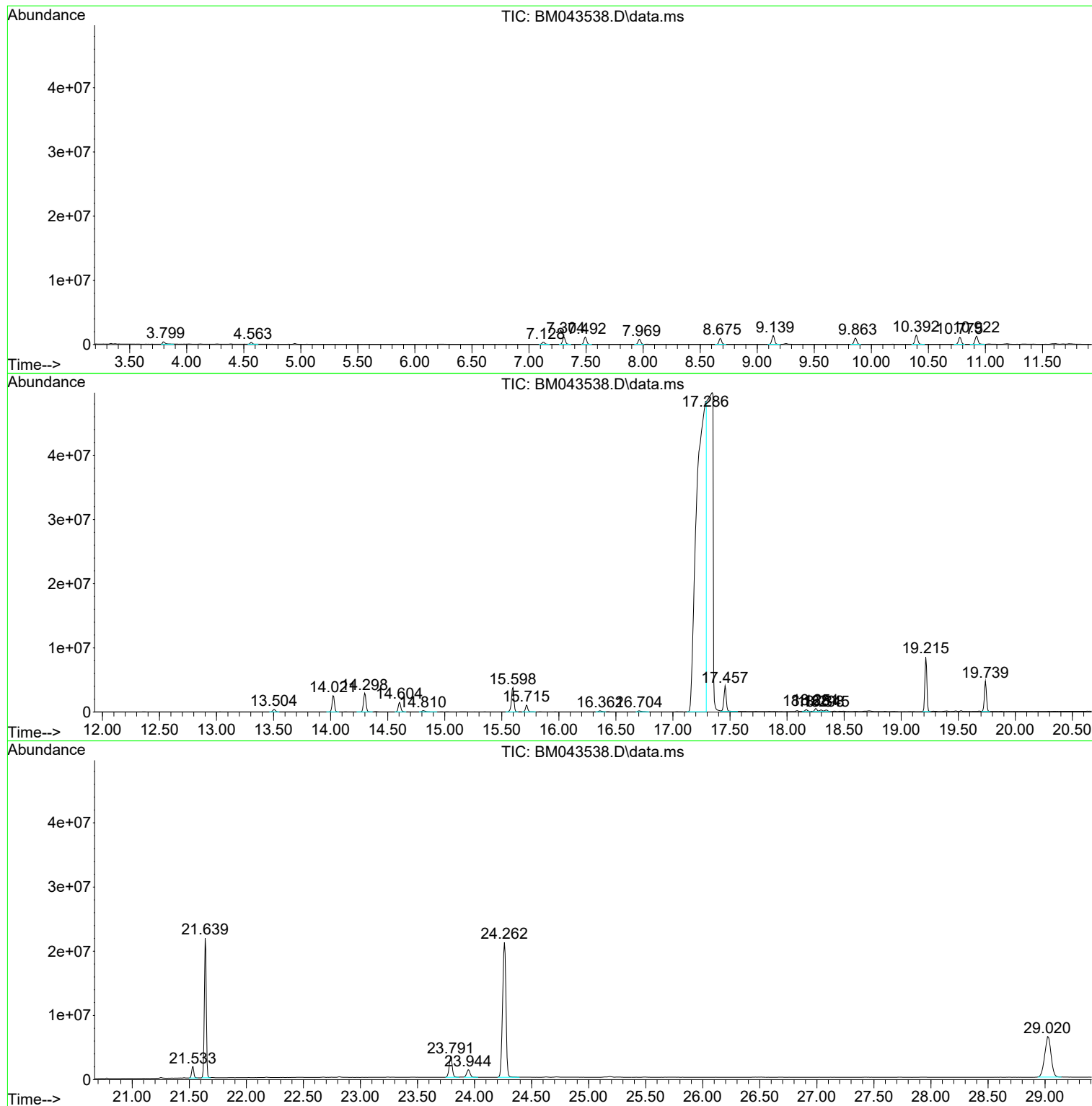
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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



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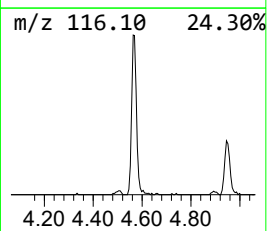
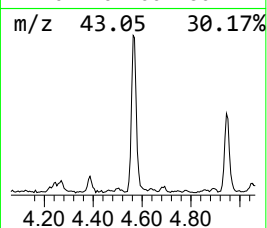
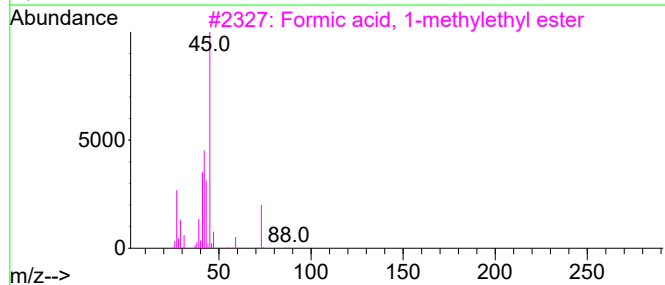
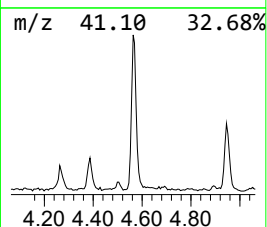
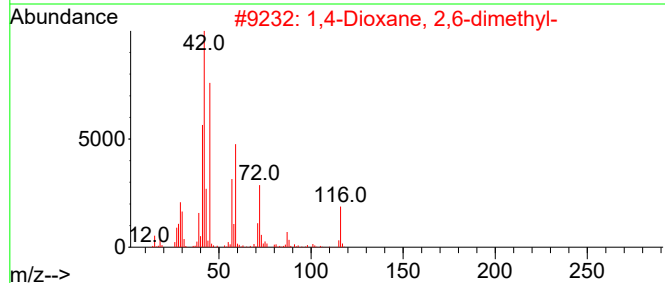
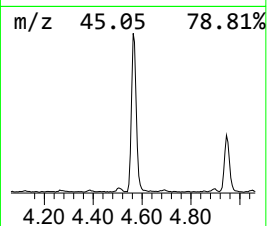
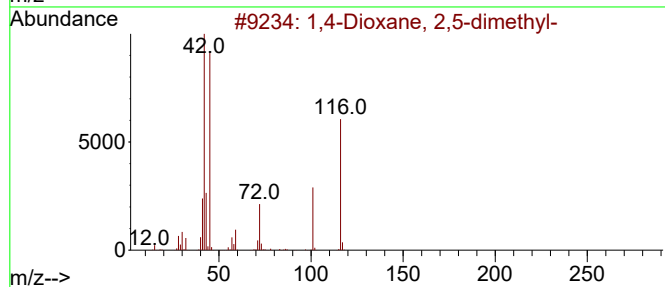
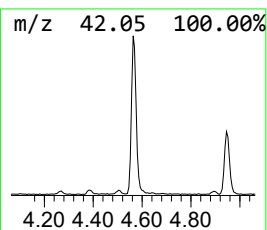
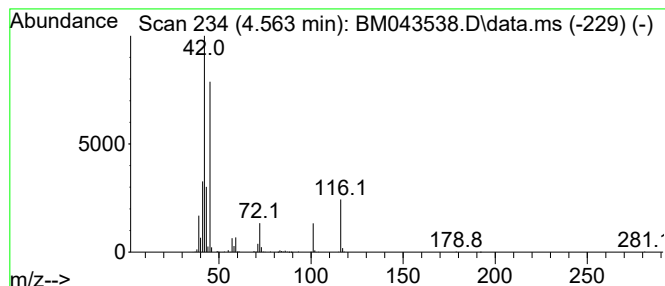
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 1,4-Dioxane, 2,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.563	6.24 ng/ul	403147	1,4-Dichlorobenzene-d4	7.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane, 2,5-dimethyl-	116	C6H12O2	015176-21-3	91		
2	1,4-Dioxane, 2,6-dimethyl-	116	C6H12O2	010138-17-7	78		
3	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	23		
4	Propane-1,3-diol, 2-methyl-	90	C4H10O2	002163-42-0	17		
5	Formic acid, propyl ester	88	C4H8O2	000110-74-7	17		



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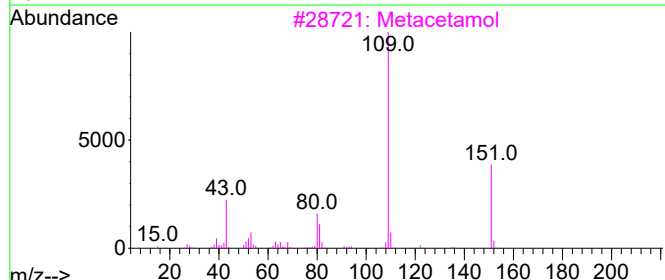
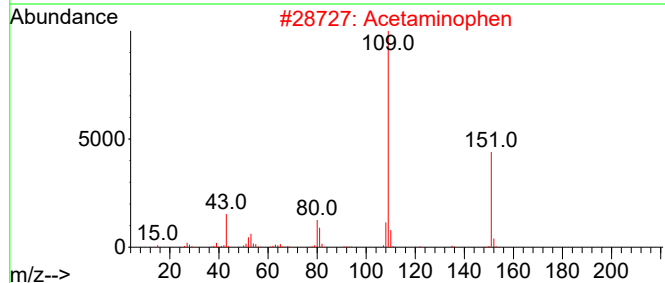
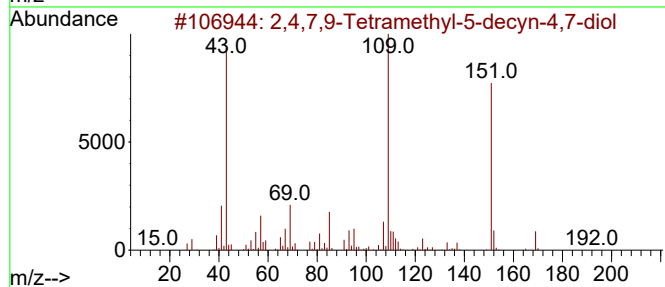
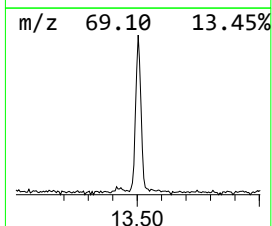
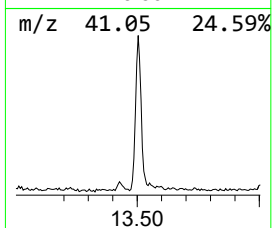
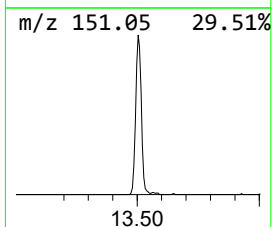
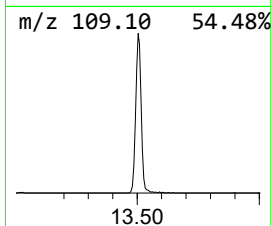
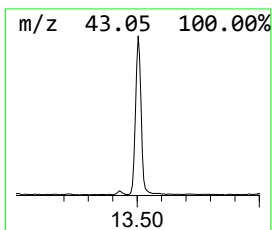
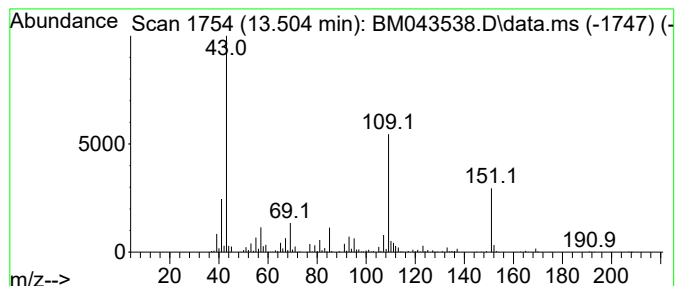
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	5.59 ng/ul	628489	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	80		
2	Acetaminophen	151	C8H9NO2	000103-90-2	46		
3	Metacetamol	151	C8H9NO2	000621-42-1	43		
4	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	43		
5	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	43		



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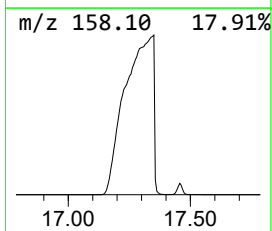
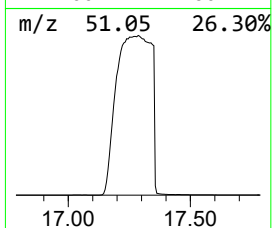
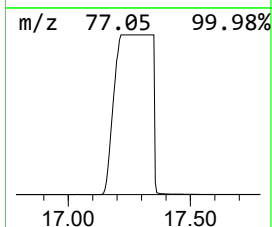
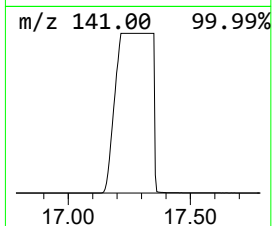
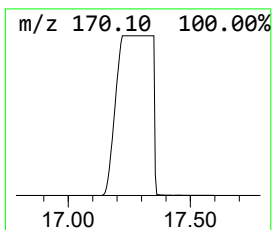
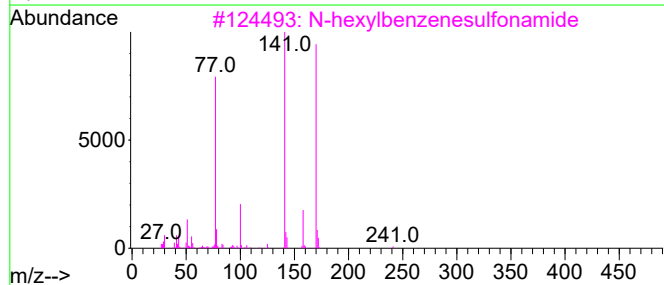
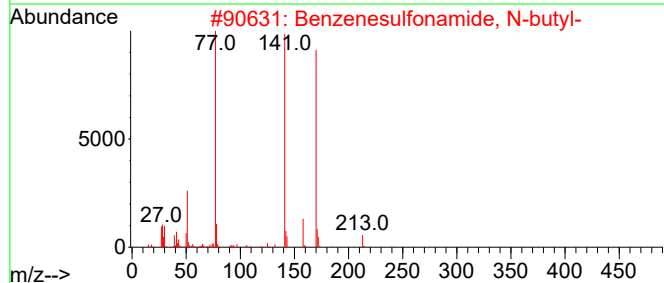
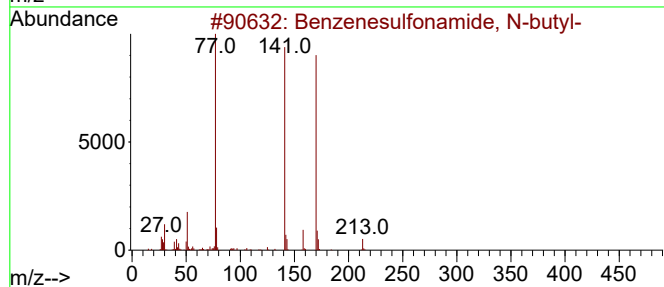
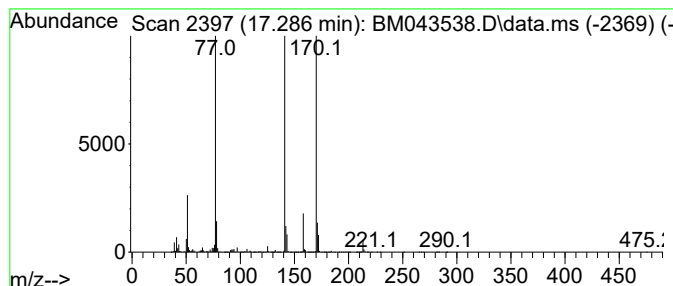
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzenesulfonamide, N-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	20.00 ng/ul	281149000	Phenanthrene-d10	17.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	97
2			Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	96
3			N-hexylbenzenesulfonamide	241	C12H19NO2S	007250-80-8	90
4			Diphenyl ether	170	C12H10O	000101-84-8	53
5			3-(Phenylsulfonyl)propanenitrile	195	C9H9NO2S	010154-75-3	47



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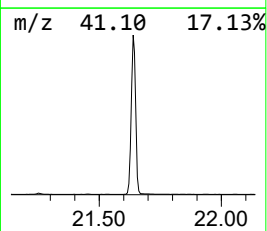
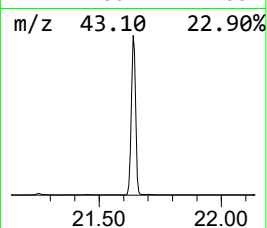
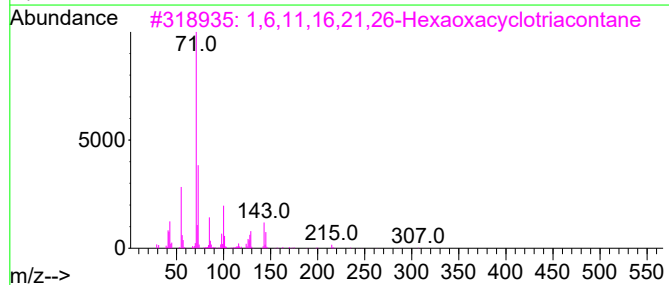
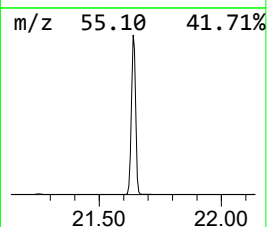
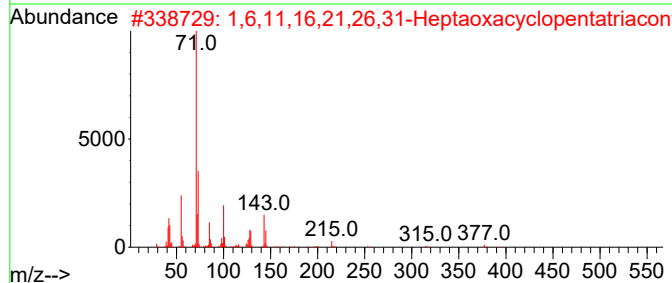
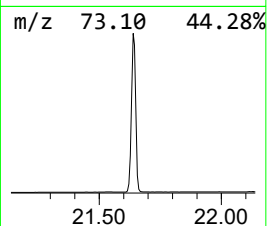
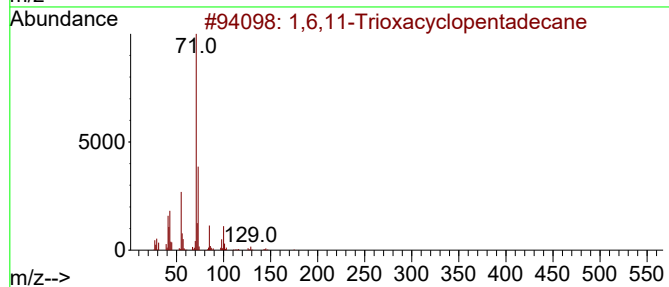
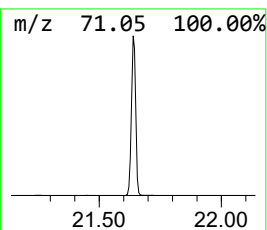
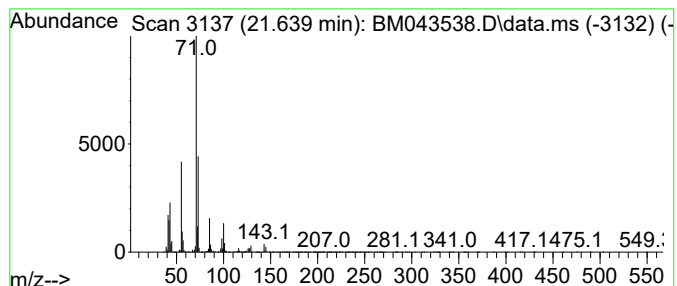
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,6,11-Trioxacyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.639	225.46 ng/ul	26407200	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	91		
2	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	74		
3	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	64		
4	3-Methoxybut-1-ene	86	C5H10O	017351-24-5	53		
5	1,6,11,16,21-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	53		



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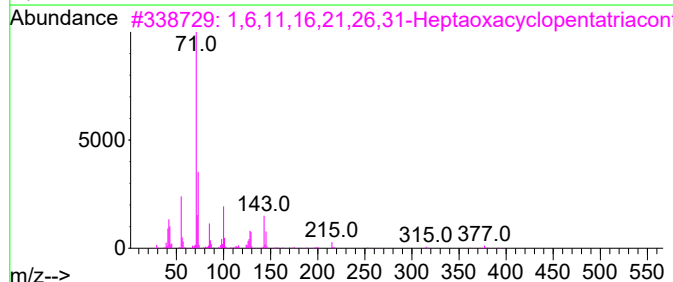
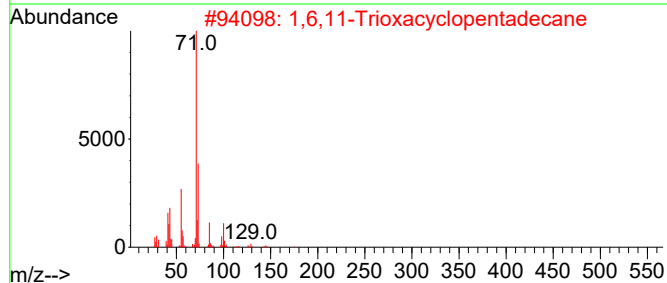
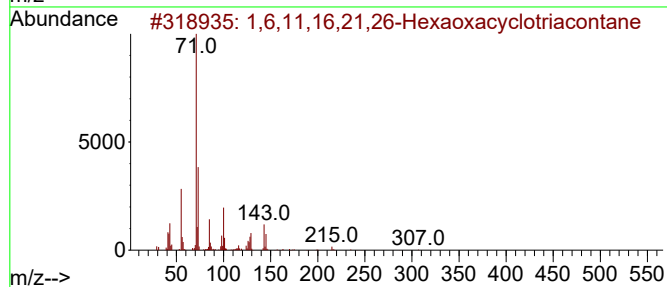
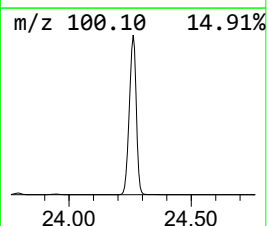
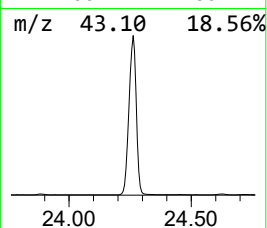
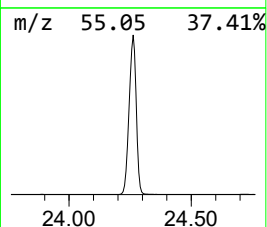
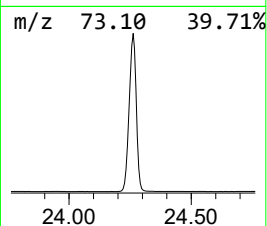
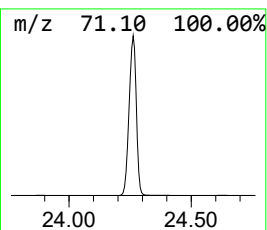
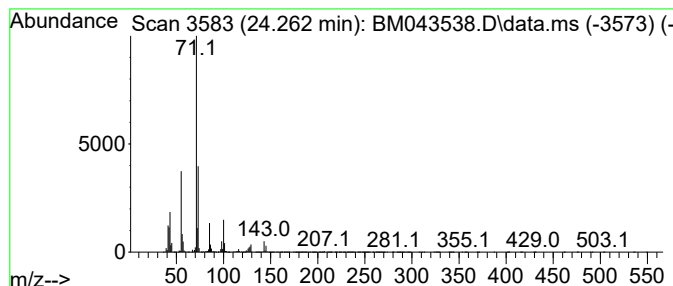
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.262	353.87 ng/ul	43531500	Perylene-d12	23.944

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	90		
3	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	52		
4	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	50		
5	Acrolein,dimethyl acetal	102	C5H10O2	006044-68-4	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
Data File : BM043538.D
Acq On : 22 Dec 2023 14:07
Operator : MA/JU
Sample : 05927-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGWA5

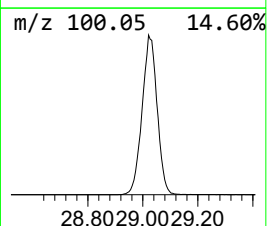
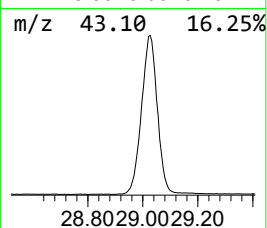
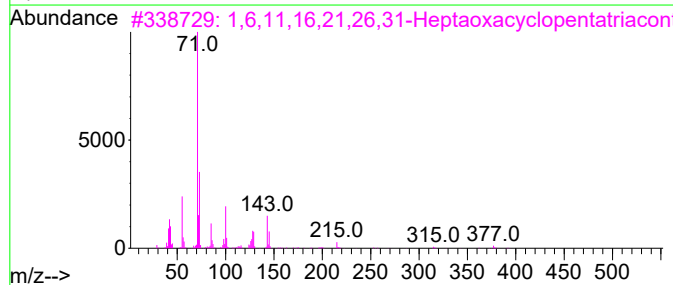
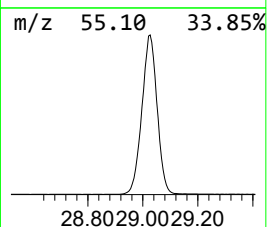
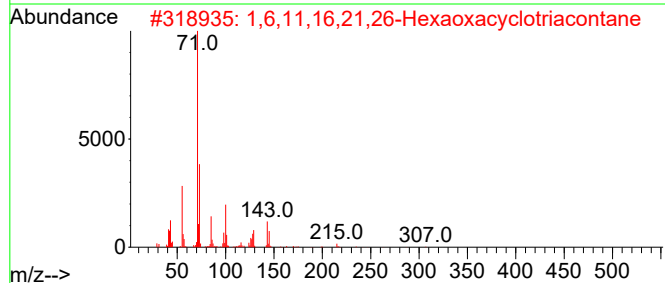
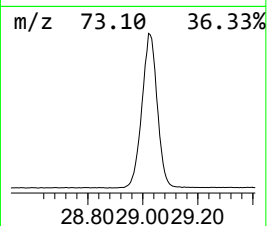
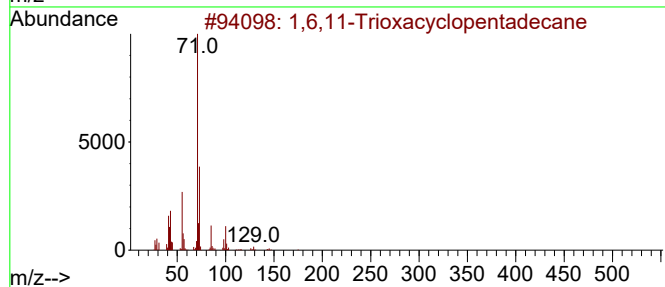
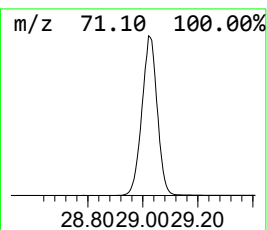
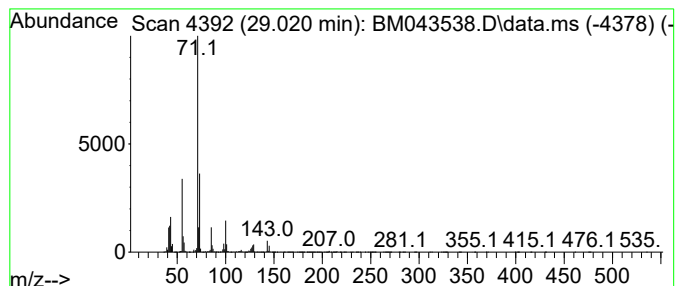
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1,6,11,16,21,26,31-Heptaoxa... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.020	197.66 ng/ul	24314900	Perylene-d12	23.944

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	1,6,11,16,21,26,31	-Heptaoxacyclo...	504	C28H56O7	066055-34-3	52	
4	Acrolein, dimethyl	acetal	102	C5H10O2	006044-68-4	47	
5	1,6,11,16,21	-Pentaoxacyclopentac...	360	C20H40O5	056890-57-4	45	



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM122123\
Data File : BM043538.D
Acq On : 22 Dec 2023 14:07
Operator : MA/JU
Sample : 05927-05
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGWA5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.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
1,4-Dioxane, 2,...	4.563	6.2	ng/ul	403147	1	7.969	1293090	20.0
2,4,7,9-Tetrame...	13.504	5.6	ng/ul	628489	3	14.604	2250100	20.0
Benzenesulfonam...	17.286	20.0	ng/ul	281149000	4	17.357	281149000	20.0
1,6,11-Trioxacy...	21.639	225.5	ng/ul	26407200	5	21.533	2342530	20.0
1,6,11,16,21,26...	24.262	353.9	ng/ul	43531500	6	23.944	2460310	20.0
1,6,11,16,21,26...	29.020	197.7	ng/ul	24314900	6	23.944	2460310	20.0