

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
 Data File : BN022814.D
 Acq On : 22 Nov 2022 08:16
 Operator : CG/JU
 Sample : N5652-13
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 BH1M2

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_N\Methods\SFAM-EPA-BN111522.M
 Title : SVOA CALIBRATION

Signal : TIC: BN022814.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	21	25	30	rBV	127598	198052	7.24%	0.748%
2	3.623	105	108	120	rBV	57101	102262	3.74%	0.386%
3	3.846	141	146	153	rVB2	9039	15415	0.56%	0.058%
4	3.940	159	162	168	rBV2	4417	6189	0.23%	0.023%
5	4.487	249	255	263	rBV	20717	34028	1.24%	0.129%
6	7.017	678	685	694	rBV	93287	149565	5.47%	0.565%
7	7.181	706	713	722	rBV	314145	495438	18.12%	1.872%
8	7.369	739	745	756	rBV	308875	503563	18.41%	1.903%
9	7.464	756	761	767	rBV3	7683	14219	0.52%	0.054%
10	7.846	817	826	835	rBV	298192	473072	17.30%	1.788%
11	8.569	943	949	962	rBV	272215	436626	15.97%	1.650%
12	9.022	1019	1026	1041	rBV	407201	673988	24.65%	2.547%
13	9.405	1085	1091	1096	rVB3	5637	9430	0.34%	0.036%
14	9.752	1142	1150	1160	rBV	331428	555768	20.32%	2.100%
15	10.287	1234	1241	1253	rBV	468658	778581	28.47%	2.942%
16	10.663	1297	1305	1313	rBV	458131	749780	27.42%	2.833%
17	10.816	1323	1331	1343	rBV	350025	644482	23.57%	2.435%
18	12.081	1542	1546	1552	rVB3	5914	9399	0.34%	0.036%
19	12.204	1557	1567	1573	rVV	54353	93446	3.42%	0.353%
20	12.263	1573	1577	1585	rVB2	7067	11867	0.43%	0.045%
21	12.893	1680	1684	1690	rVB4	2713	3714	0.14%	0.014%
22	13.034	1705	1708	1713	rVB4	2805	3934	0.14%	0.015%
23	13.328	1753	1758	1766	rVV	13265	19655	0.72%	0.074%
24	13.410	1766	1772	1778	rVB5	2591	4290	0.16%	0.016%
25	13.934	1850	1861	1875	rBV	973740	1332433	48.73%	5.035%
26	14.034	1875	1878	1883	rVB2	2355	3609	0.13%	0.014%
27	14.210	1901	1908	1923	rBV	1052761	1516246	55.45%	5.729%
28	14.404	1937	1941	1945	rBV2	4110	5869	0.21%	0.022%
29	14.516	1953	1960	1968	rBV	744134	1049946	38.40%	3.967%
30	14.740	1992	1998	2017	rBV	67891	146627	5.36%	0.554%
31	14.951	2032	2034	2039	rVB2	4437	5127	0.19%	0.019%
32	15.040	2044	2049	2052	rVB4	1710	2914	0.11%	0.011%
33	15.357	2097	2103	2107	rVB4	2828	4463	0.16%	0.017%
34	15.510	2117	2129	2144	rBV	1372003	2017183	73.77%	7.622%
35	15.645	2146	2152	2168	rBV	521507	720874	26.36%	2.724%
36	15.751	2168	2170	2173	rVB2	5207	5234	0.19%	0.020%

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37	15.881	2188	2192	2197	rBV	8694	11938	0.44%	0.045%
38	16.040	2213	2219	2224	rBV2	3496	4710	0.17%	0.018%
39	16.557	2304	2307	2314	rVB4	2537	4310	0.16%	0.016%
40	16.781	2341	2345	2351	rBV4	4313	6657	0.24%	0.025%
41	17.063	2388	2393	2400	rVB5	2100	3863	0.14%	0.015%
42	17.269	2422	2428	2435	rBV	927177	1277435	46.71%	4.827%
43	17.369	2439	2445	2455	rVV2	1568962	2187721	80.00%	8.267%
44	17.451	2455	2459	2466	rVB2	20869	29340	1.07%	0.111%
45	17.551	2473	2476	2481	rBV4	2370	3529	0.13%	0.013%
46	17.663	2489	2495	2497	rBV4	2524	4171	0.15%	0.016%
47	17.939	2539	2542	2547	rVB4	2821	3028	0.11%	0.011%
48	18.039	2554	2559	2562	rBV4	2674	4307	0.16%	0.016%
49	18.163	2575	2580	2589	rBV	88285	125481	4.59%	0.474%
50	18.245	2591	2594	2601	rVB2	4825	8894	0.33%	0.034%
51	18.357	2609	2613	2618	rVB5	3333	5509	0.20%	0.021%
52	18.592	2648	2653	2658	rBV	34385	41126	1.50%	0.155%
53	18.734	2674	2677	2684	rVB5	2341	4356	0.16%	0.016%
54	19.134	2740	2745	2750	rBV	245421	304300	11.13%	1.150%
55	19.233	2758	2762	2769	rVB2	19762	26116	0.96%	0.099%
56	19.310	2770	2775	2780	rBV	21628	35248	1.29%	0.133%
57	19.386	2784	2788	2794	rVB	100471	112124	4.10%	0.424%
58	19.445	2794	2798	2806	rBV	41060	58055	2.12%	0.219%
59	19.592	2820	2823	2829	rVB3	6675	9185	0.34%	0.035%
60	19.675	2830	2837	2848	rBV	1986277	2586373	94.58%	9.773%
61	20.604	2992	2995	2998	rBV4	5542	7108	0.26%	0.027%
62	20.704	3010	3012	3017	rBV4	7391	7760	0.28%	0.029%
63	21.186	3088	3094	3106	rBV2	110324	271642	9.93%	1.026%
64	21.380	3124	3127	3130	rVB	24153	25639	0.94%	0.097%
65	21.475	3137	3143	3152	rBV	1119727	1438442	52.60%	5.435%
66	21.563	3153	3158	3162	rBV	344854	397235	14.53%	1.501%
67	22.563	3325	3328	3334	rVB2	43205	54811	2.00%	0.207%
68	23.116	3418	3422	3427	rVB	56299	85510	3.13%	0.323%
69	23.710	3515	3523	3536	rVB2	1281507	2734556	100.00%	10.333%
70	23.863	3542	3549	3559	rVB2	694023	1392508	50.92%	5.262%
71	24.121	3588	3593	3599	rVB	127227	235942	8.63%	0.892%
72	24.457	3645	3650	3658	rVB2	78843	157744	5.77%	0.596%

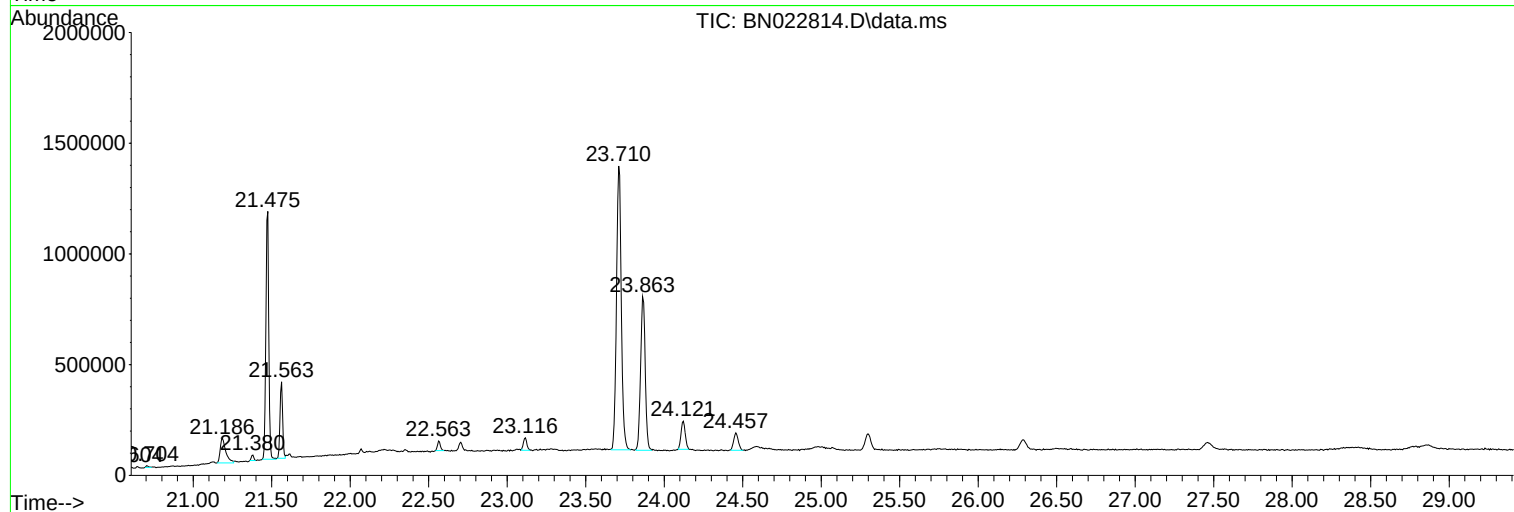
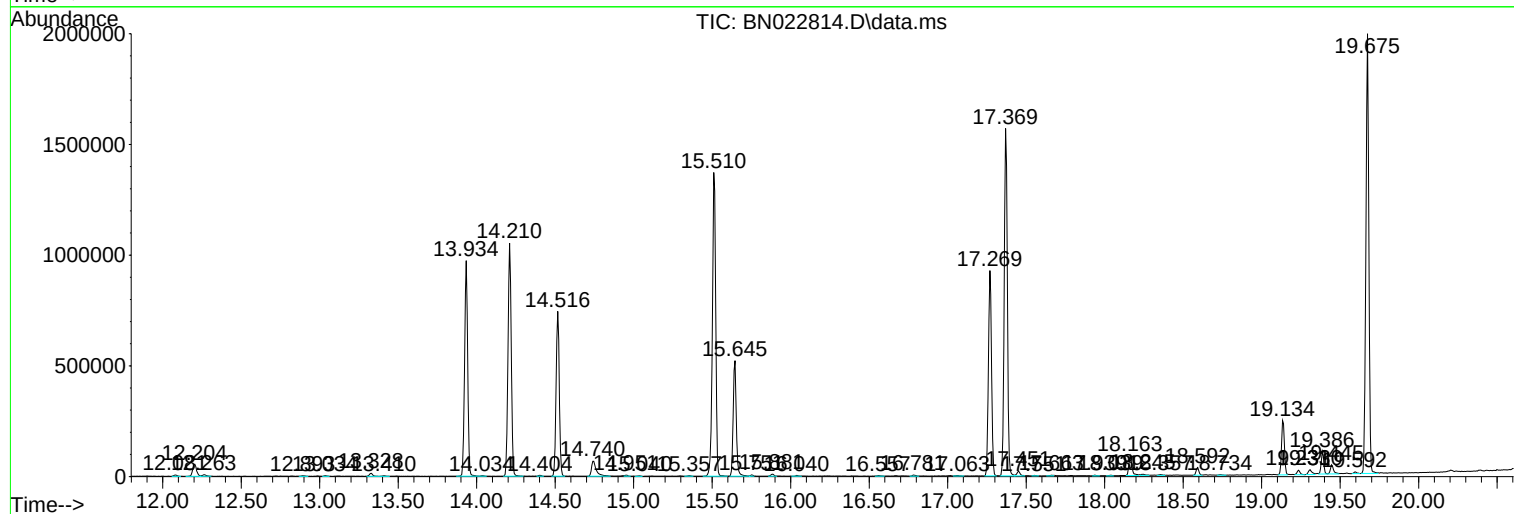
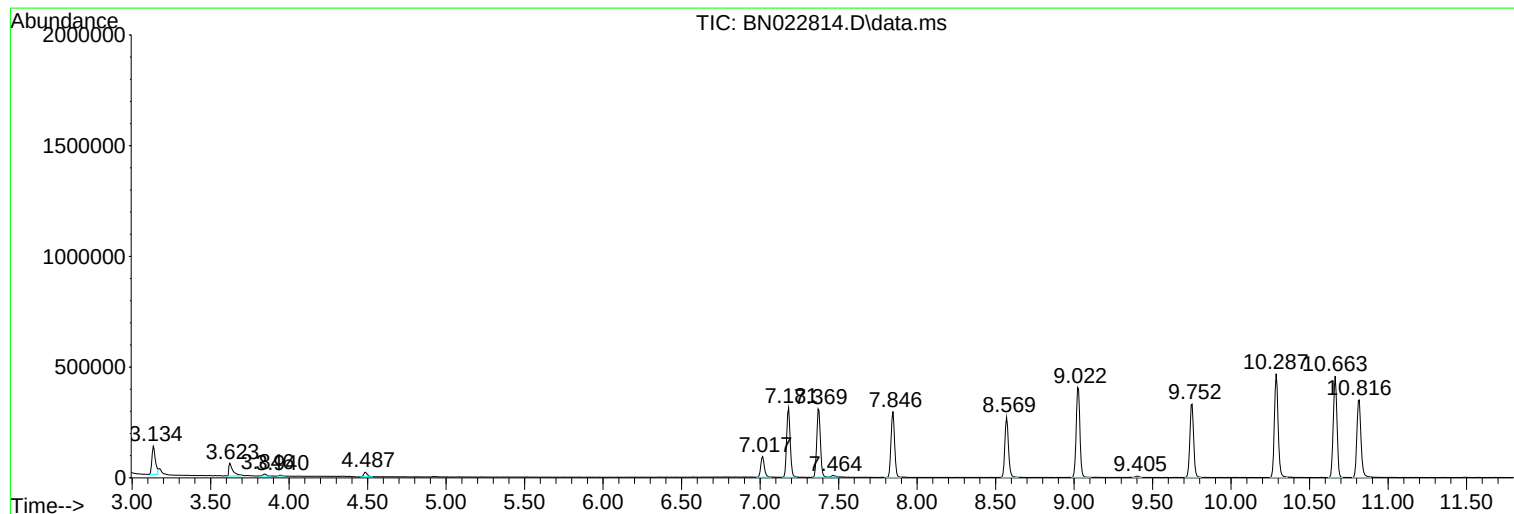
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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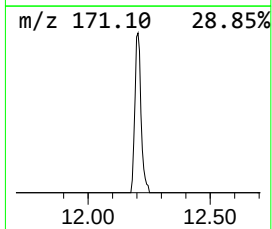
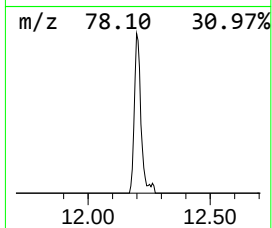
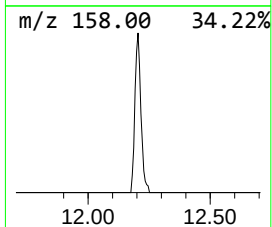
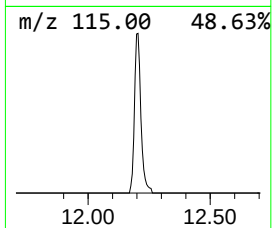
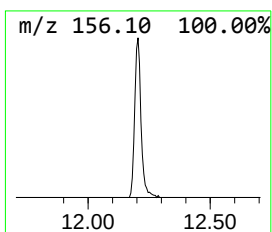
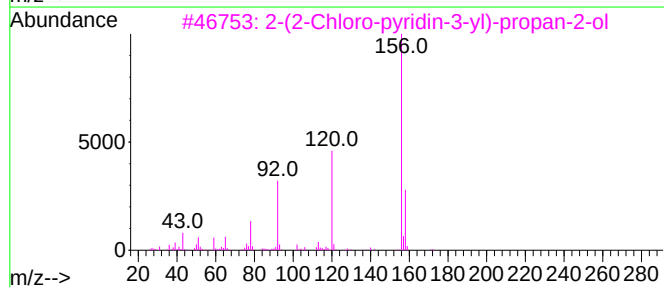
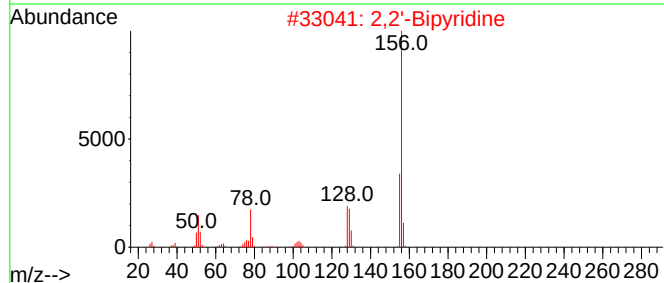
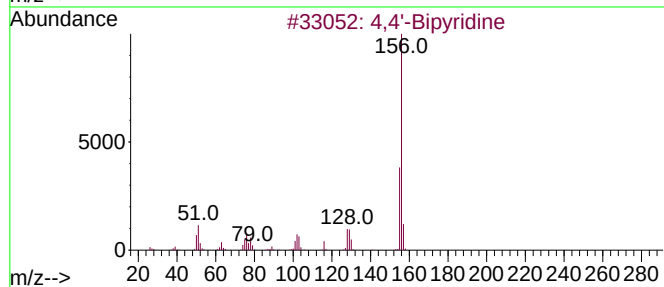
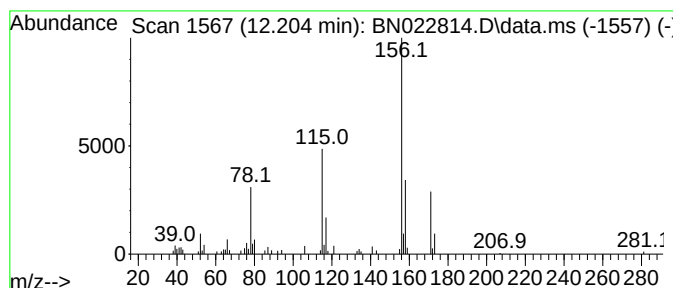
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.204	2.49 ng/ul	93446	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Bipyridine	156	C10H8N2	000553-26-4	35
2			2,2'-Bipyridine	156	C10H8N2	000366-18-7	25
3			2-(2-Chloro-pyridin-3-yl)-propan...	171	C8H10ClNO	267003-35-0	25
4			Tebuthiuron	228	C9H16N4OS	034014-18-1	25
5			4-Chloro-3,5-dimethylphenol, O-i...	242	C12H15ClO3	1000487-39-3	23



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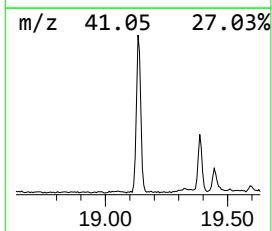
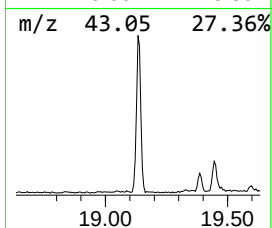
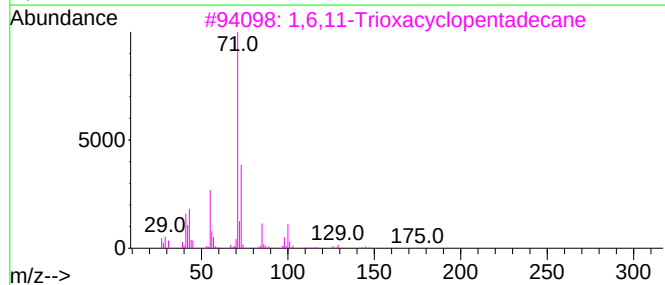
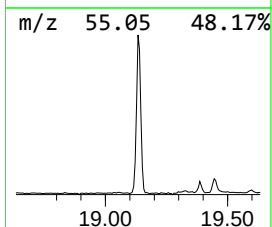
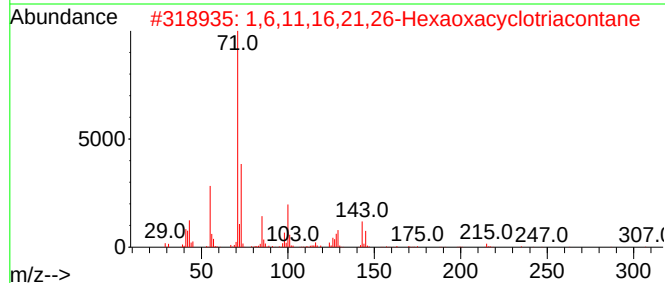
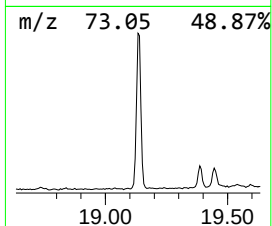
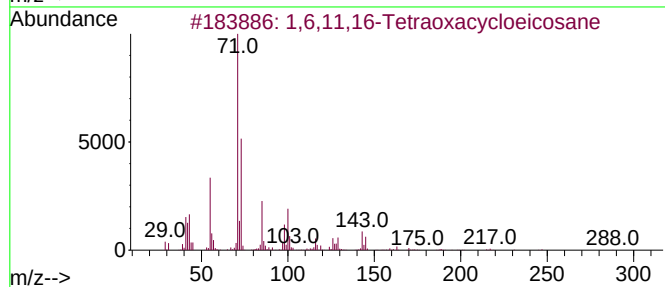
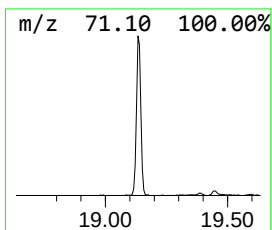
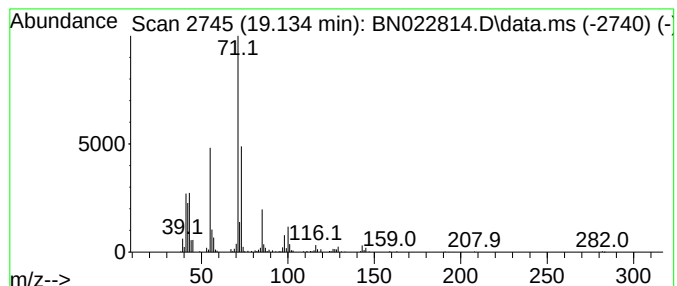
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 1,6,11,16-Tetraoxacycloeico... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.134	4.76 ng/ul	304300	Phenanthrene-d10	17.269	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	83
2	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	80
3	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	80
4	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	72
5	4-Heptanone, 3-methyl-	128	C8H16O	015726-15-5	59



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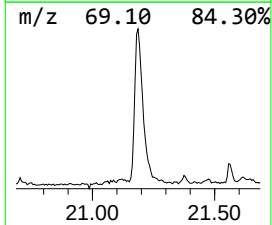
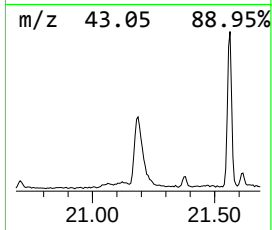
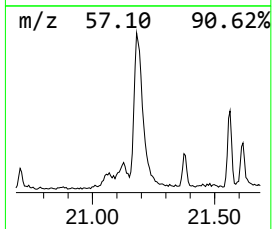
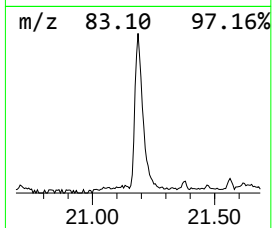
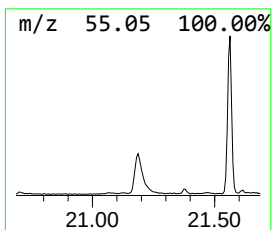
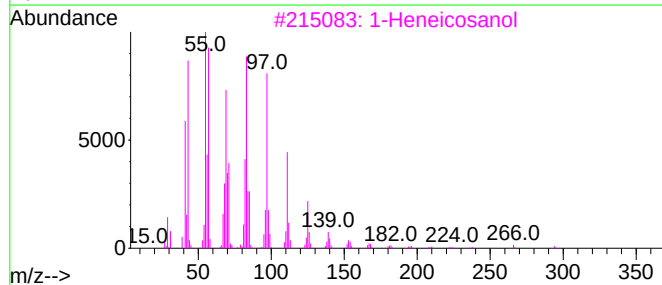
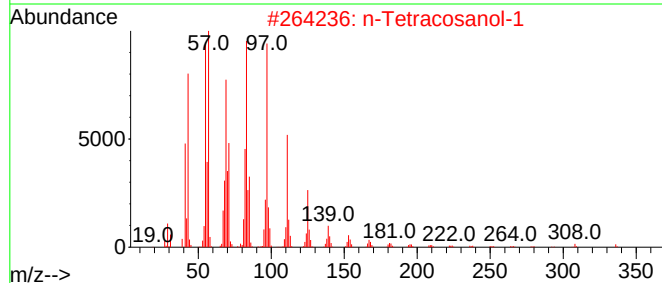
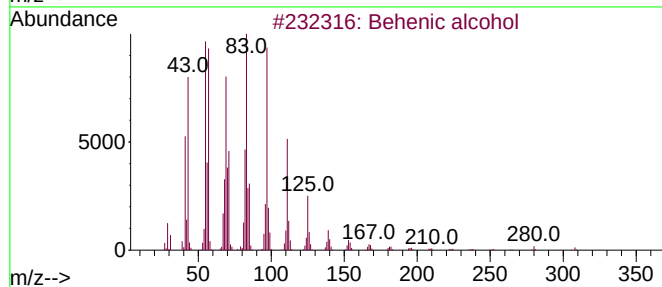
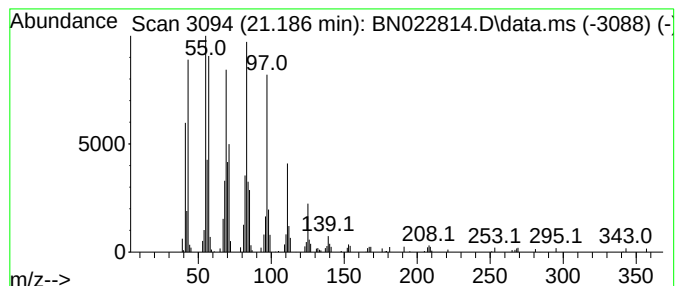
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Peak Number 3 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	3.78 ng/ul	271642	Chrysene-d12	21.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3			1-Heneicosanol	312	C21H44O	015594-90-8	95
4			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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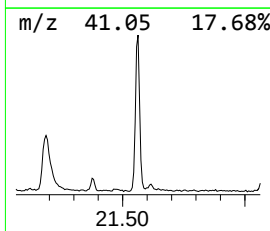
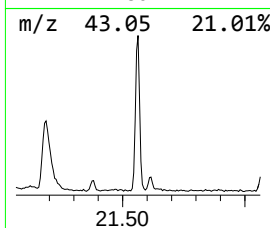
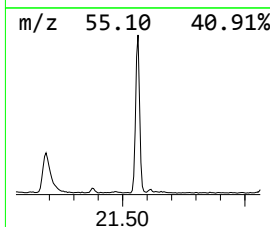
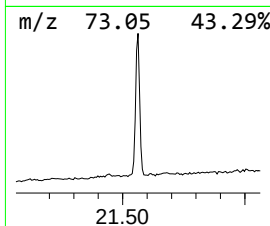
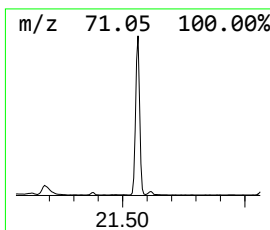
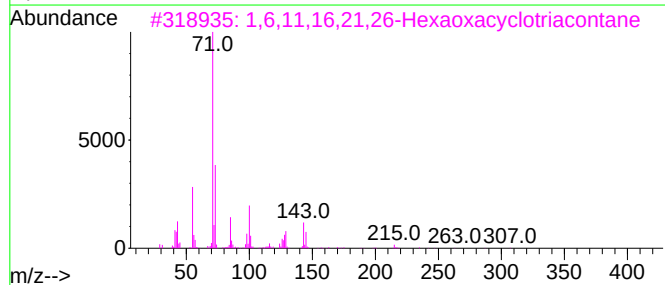
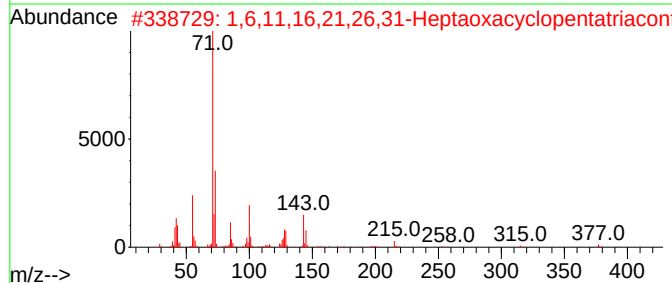
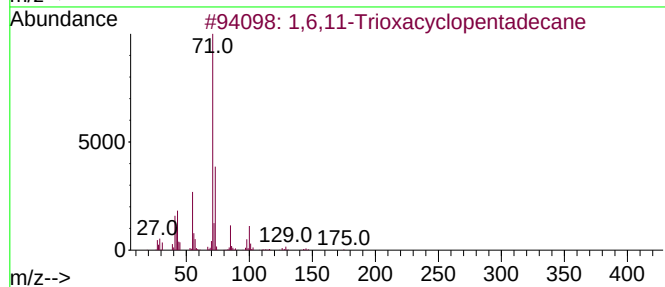
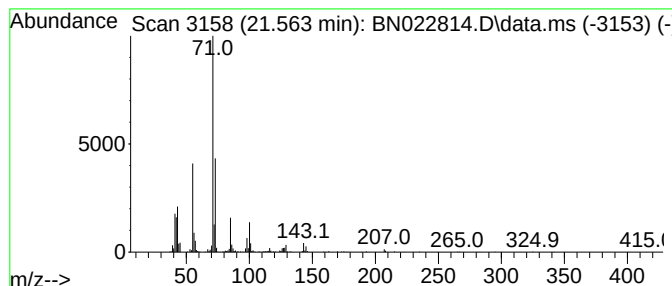
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	5.52 ng/ul	397235	Chrysene-d12	21.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6,11-Trioxacyclopentadecane	216	C12H24O3	000295-63-6	86		
2	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	83		
3	1,6,11,16,21,26-Hexaoxacyclotria...	432	C24H48O6	064001-05-4	62		
4	Acrolein,dimethyl acetal	102	C5H10O2	006044-68-4	47		
5	3-Tetrahydro-2-furanylpropanoic ...	144	C7H12O3	000935-12-6	42		



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Data File : BN022814.D
Acq On : 22 Nov 2022 08:16
Operator : CG/JU
Sample : N5652-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BH1M2

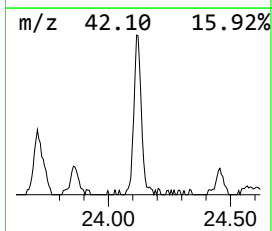
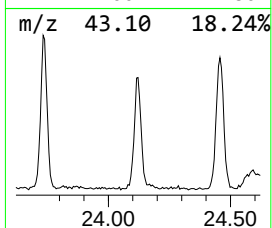
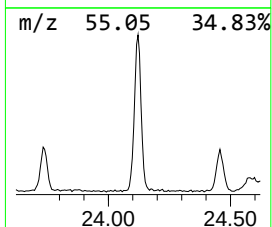
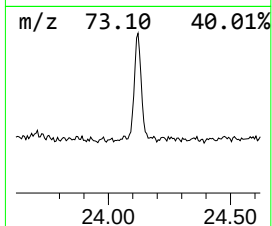
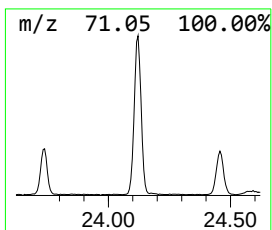
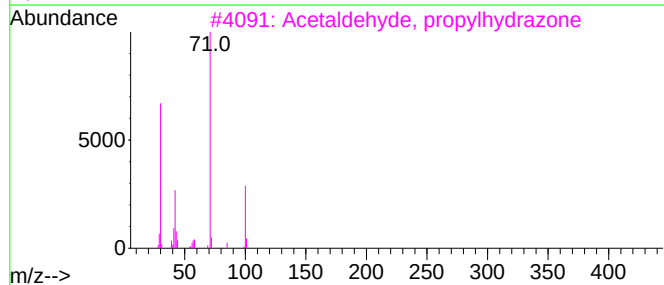
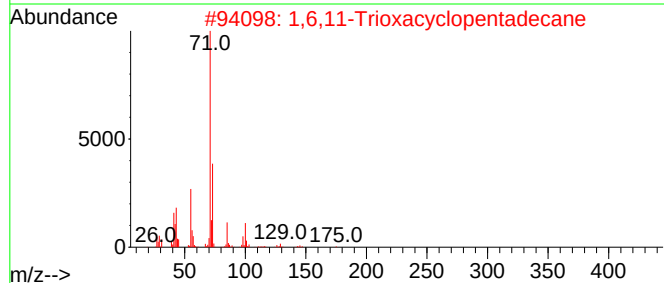
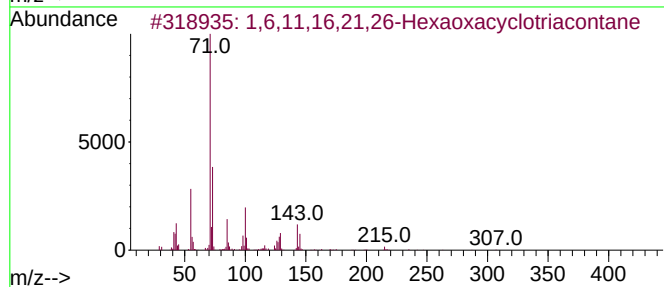
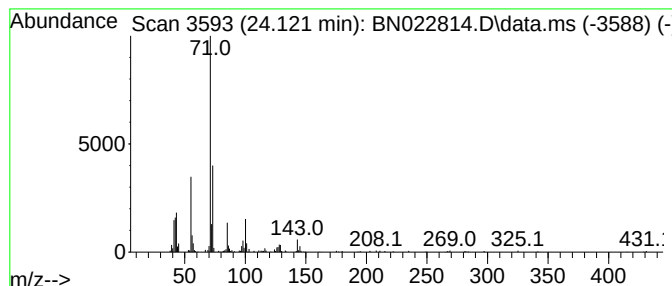
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1,6,11,16,21,26-Hexaoxacycl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.122	3.39 ng/ul	235942	Perylene-d12	23.863

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	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	58		
4	1,6,11,16,21,26,31-Heptaoxacyclo...	504	C28H56O7	066055-34-3	53		
5	1,6,11,16-Tetraoxacycloeicosane	288	C16H32O4	017043-02-6	50		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
Data File : BN022814.D
Acq On : 22 Nov 2022 08:16
Operator : CG/JU
Sample : N5652-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
BH1M2

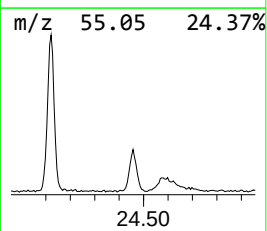
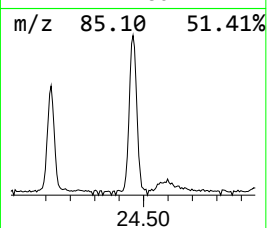
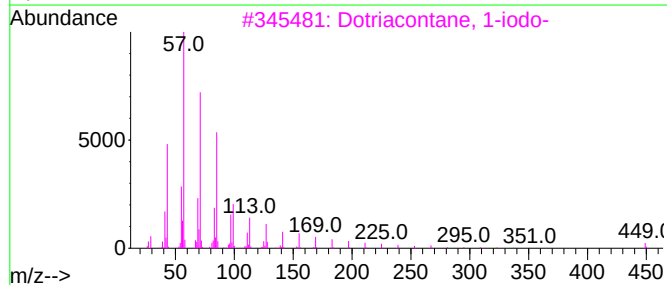
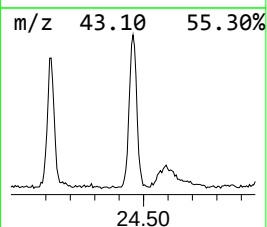
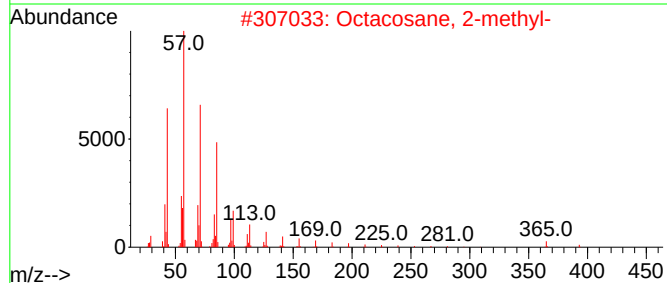
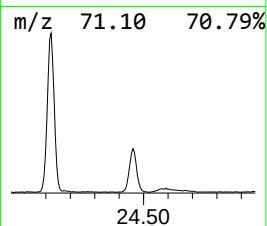
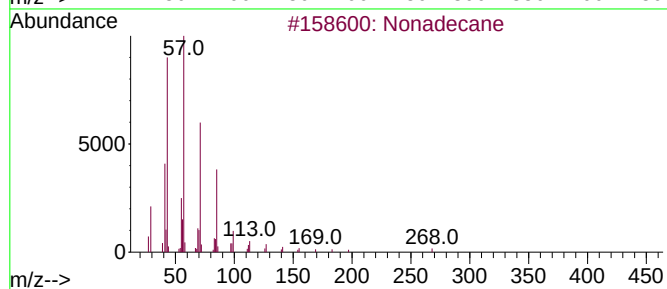
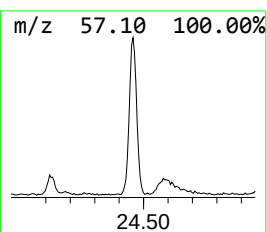
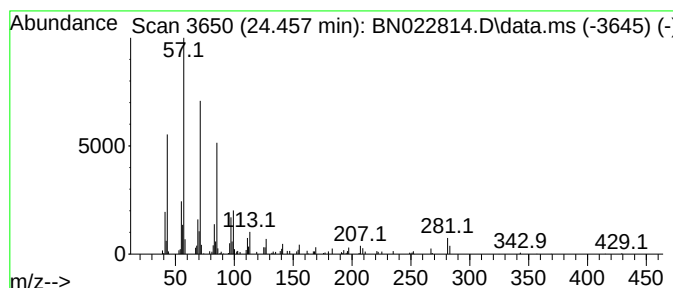
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.457	2.27 ng/ul	157744	Perylene-d12	23.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
4			Heptacosane	380	C27H56	000593-49-7	87
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
Data File : BN022814.D
Acq On : 22 Nov 2022 08:16
Operator : CG/JU
Sample : N5652-13
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
BH1M2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.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
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1,6,11,16-Tetra...	19.134	4.8	ng/ul	304300	4	17.269	1277440	20.0
Behenic alcohol	21.186	3.8	ng/ul	271642	5	21.475	1438440	20.0
1,6,11-Trioxacy...	21.563	5.5	ng/ul	397235	5	21.475	1438440	20.0
1,6,11,16,21,26...	24.122	3.4	ng/ul	235942	6	23.863	1392510	20.0
(DEL) Alkane: S...	24.457	2.3	ng/ul	157744	6	23.863	1392510	20.0