

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
 Data File : BN022833.D
 Acq On : 22 Nov 2022 20:21
 Operator : CG/JU
 Sample : N5593-10
 Misc :
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 H0AD9

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: BN022833.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	29	rBV	14404	21296	0.80%	0.086%
2	3.175	29	32	36	rVV	16815	22831	0.85%	0.092%
3	3.211	36	38	45	rVB	14711	20366	0.76%	0.082%
4	3.617	105	107	125	rBV	98530	179913	6.72%	0.727%
5	3.840	142	145	151	rVB	7427	10958	0.41%	0.044%
6	3.940	160	162	169	rVB2	4620	6876	0.26%	0.028%
7	4.487	249	255	271	rVB	110253	189498	7.08%	0.766%
8	4.917	323	328	343	rVB	19648	34628	1.29%	0.140%
9	7.016	679	685	697	rVB	95100	157241	5.88%	0.635%
10	7.181	706	713	723	rBV	319168	506351	18.92%	2.046%
11	7.369	738	745	756	rBV	315016	516773	19.31%	2.088%
12	7.446	756	758	763	rVB3	2019	2685	0.10%	0.011%
13	7.846	820	826	838	rBV	247484	401622	15.01%	1.623%
14	8.569	943	949	963	rBV	280564	460583	17.21%	1.861%
15	9.022	1020	1026	1040	rVV	414192	685350	25.61%	2.769%
16	9.369	1081	1085	1089	rBV5	2790	5101	0.19%	0.021%
17	9.746	1142	1149	1160	rBV	343342	576402	21.54%	2.329%
18	10.222	1222	1230	1234	rBV5	2424	4717	0.18%	0.019%
19	10.287	1234	1241	1259	rVV	475448	809422	30.25%	3.271%
20	10.663	1294	1305	1312	rBV	384947	636469	23.78%	2.572%
21	10.716	1312	1314	1322	rVB3	3192	5097	0.19%	0.021%
22	10.816	1322	1331	1343	rBV	404364	729033	27.24%	2.946%
23	11.475	1436	1443	1448	rBV5	2928	6043	0.23%	0.024%
24	11.881	1508	1512	1523	rVB4	1674	4418	0.17%	0.018%
25	12.175	1558	1562	1568	rBV5	2122	3342	0.12%	0.014%
26	12.234	1568	1572	1573	rVV4	3230	4236	0.16%	0.017%
27	12.263	1574	1577	1585	rVB2	6165	10957	0.41%	0.044%
28	13.404	1767	1771	1779	rBV5	3124	5390	0.20%	0.022%
29	13.934	1851	1861	1868	rBV	988901	1356350	50.68%	5.481%
30	14.045	1876	1880	1885	rBV5	1799	2965	0.11%	0.012%
31	14.210	1901	1908	1919	rBV	1078631	1531060	57.21%	6.187%
32	14.440	1942	1947	1952	rBV2	26362	35980	1.34%	0.145%
33	14.516	1954	1960	1968	rVB	590247	858922	32.10%	3.471%
34	14.740	1993	1998	2014	rBV	88652	171454	6.41%	0.693%
35	14.992	2037	2041	2047	rBV8	2367	4579	0.17%	0.019%
36	15.269	2082	2088	2091	rBV	7451	11108	0.42%	0.045%

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37	15.340	2097	2100	2105	rVB3	8031	10945	0.41%	0.044%
38	15.510	2123	2129	2142	rBV	1325524	1916019	71.60%	7.742%
39	15.645	2145	2152	2166	rVV	545783	759107	28.37%	3.067%
40	15.751	2166	2170	2180	rVB5	6980	17459	0.65%	0.071%
41	16.034	2210	2218	2223	rBV	34269	48283	1.80%	0.195%
42	16.139	2233	2236	2241	rVB4	3145	4203	0.16%	0.017%
43	16.216	2244	2249	2260	rVV	69285	110749	4.14%	0.448%
44	16.298	2260	2263	2267	rVB5	3707	6067	0.23%	0.025%
45	16.551	2302	2306	2311	rBV	16442	21882	0.82%	0.088%
46	16.669	2322	2326	2330	rVB5	2862	3835	0.14%	0.015%
47	16.798	2342	2348	2350	rBV6	2196	4011	0.15%	0.016%
48	17.057	2388	2392	2395	rBV6	3196	4214	0.16%	0.017%
49	17.269	2422	2428	2438	rVB	743233	1036729	38.74%	4.189%
50	17.369	2438	2445	2455	rBV	1492971	2159899	80.71%	8.728%
51	17.586	2477	2482	2484	rBV4	2333	3466	0.13%	0.014%
52	17.616	2485	2487	2490	rVV2	3107	3775	0.14%	0.015%
53	17.816	2518	2521	2524	rVB5	2620	2877	0.11%	0.012%
54	17.939	2538	2542	2544	rBV3	4226	4380	0.16%	0.018%
55	18.163	2575	2580	2588	rBV	48861	71878	2.69%	0.290%
56	18.245	2590	2594	2596	rBV2	10048	13664	0.51%	0.055%
57	18.463	2627	2631	2634	rVB6	1996	3130	0.12%	0.013%
58	18.516	2636	2640	2644	rBV7	3232	5311	0.20%	0.021%
59	18.681	2663	2668	2671	rBV6	2885	4371	0.16%	0.018%
60	19.233	2759	2762	2768	rBV2	19023	26573	0.99%	0.107%
61	19.304	2770	2774	2780	rBV	22330	35977	1.34%	0.145%
62	19.386	2783	2788	2794	rVV	492939	556260	20.79%	2.248%
63	19.445	2794	2798	2806	rVB2	32933	46068	1.72%	0.186%
64	19.592	2821	2823	2830	rVB6	6560	7936	0.30%	0.032%
65	19.675	2830	2837	2848	rBV	1938774	2522850	94.27%	10.194%
66	21.192	3092	3095	3101	rVB4	34446	55143	2.06%	0.223%
67	21.469	3137	3142	3154	rBV	847414	1133869	42.37%	4.582%
68	22.563	3325	3328	3333	rVB2	32820	43253	1.62%	0.175%
69	23.110	3418	3421	3426	rVB	52879	77854	2.91%	0.315%
70	23.710	3515	3523	3539	rVB2	1308256	2676085	100.00%	10.814%
71	23.863	3542	3549	3560	rVB2	533845	1069286	39.96%	4.321%
72	24.457	3645	3650	3657	rVB3	69805	145291	5.43%	0.587%
73	25.292	3789	3792	3802	rVB	65414	144602	5.40%	0.584%

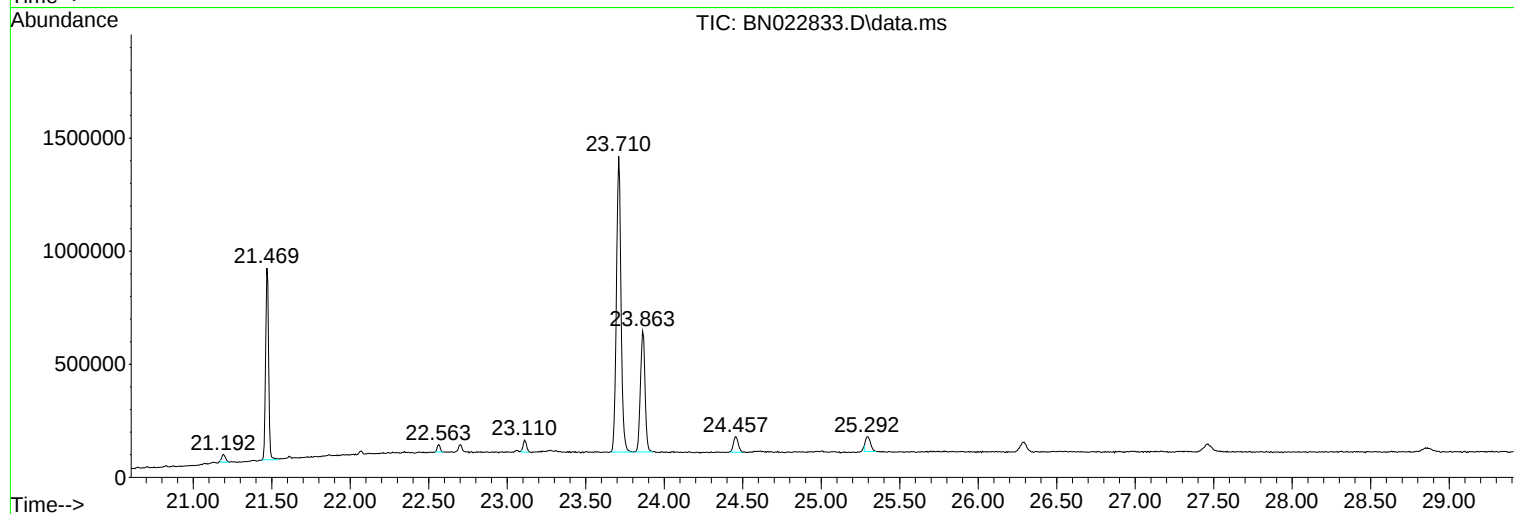
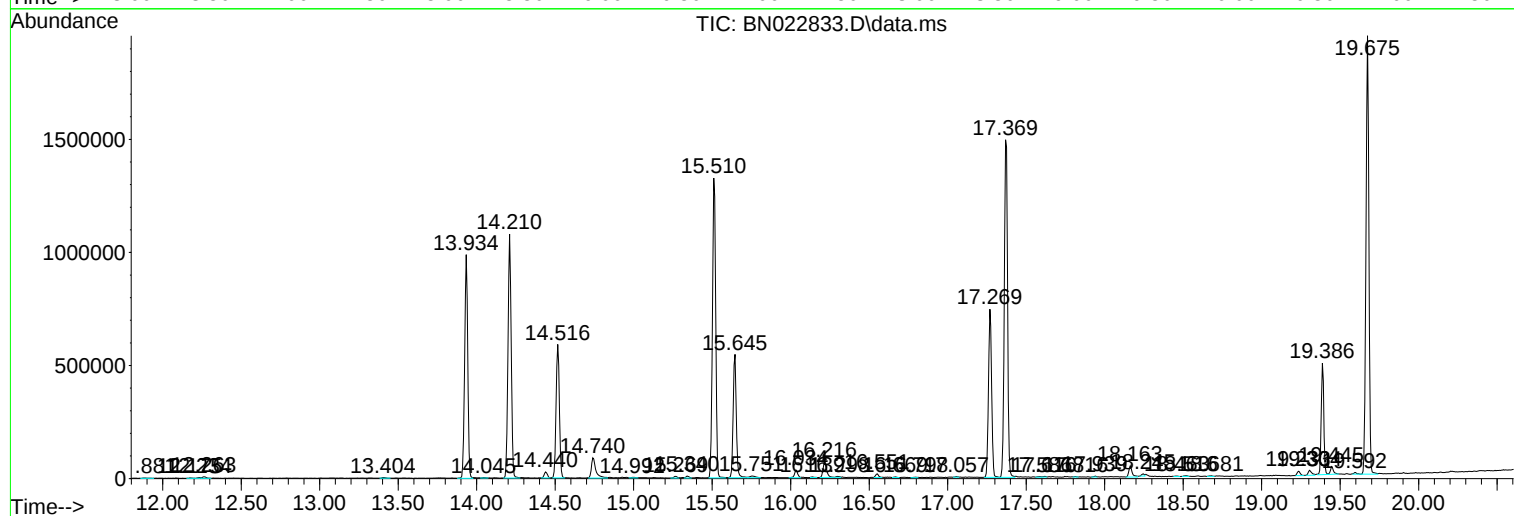
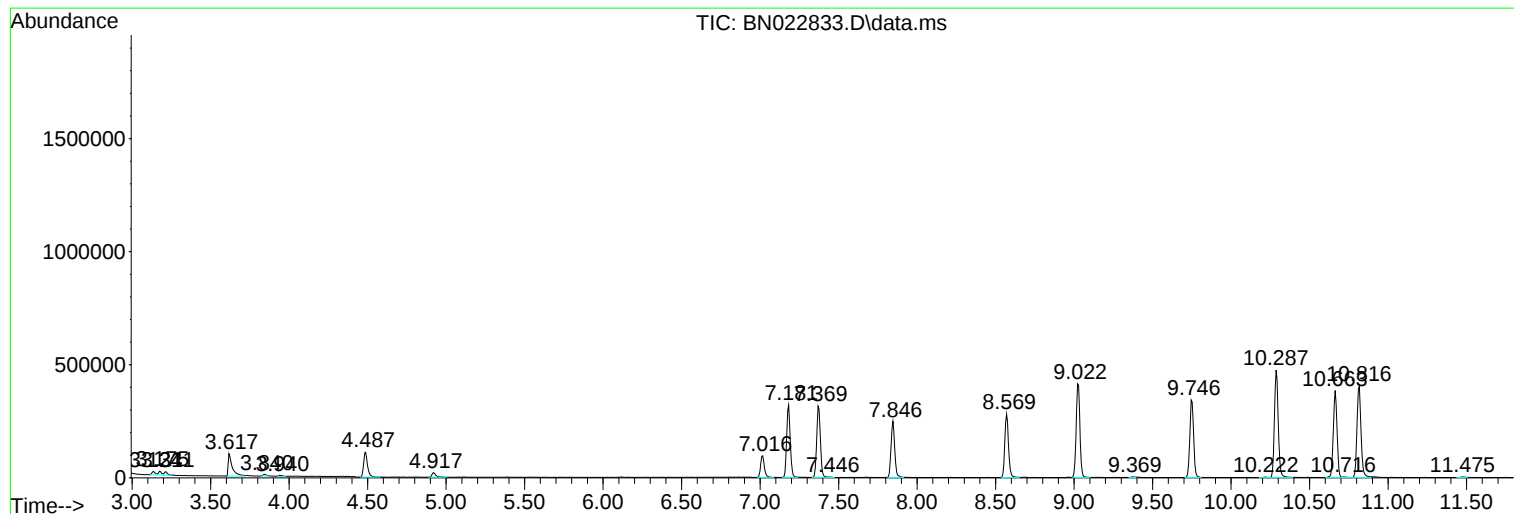
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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



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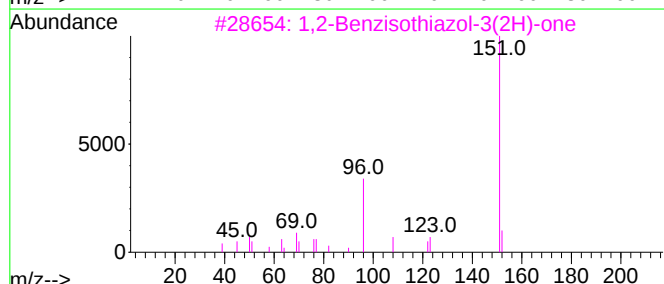
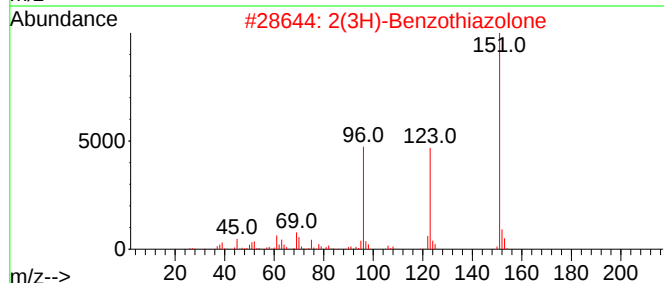
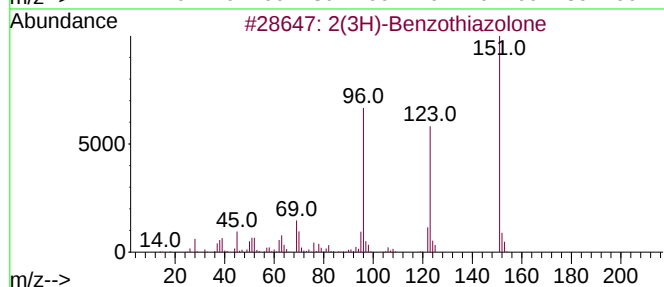
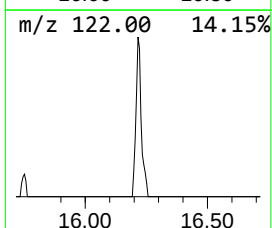
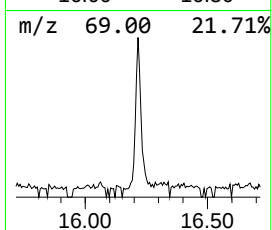
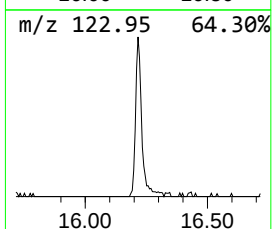
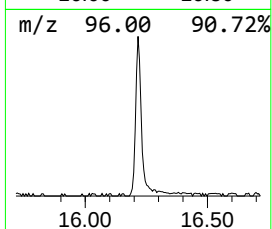
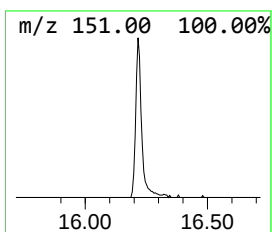
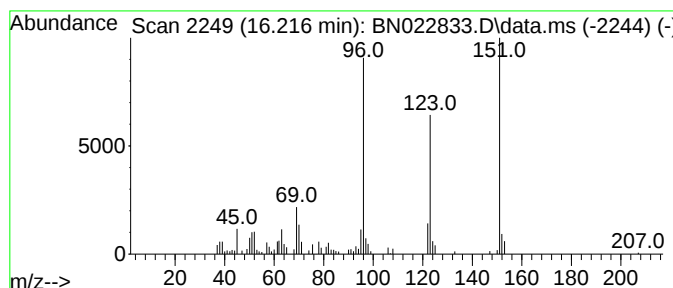
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 2(3H)-Benzothiazolone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.216	2.14 ng/ul	110749	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	96
2			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	94
3			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	76
4			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	49
5			Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	43



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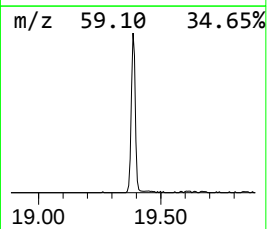
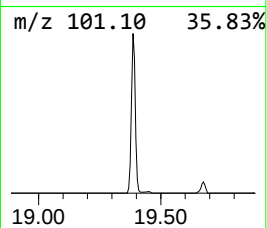
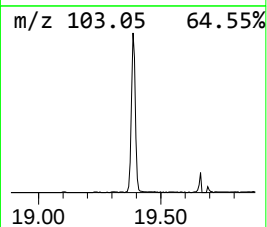
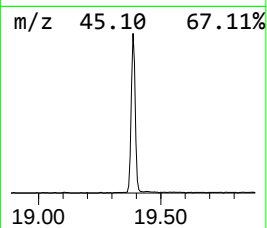
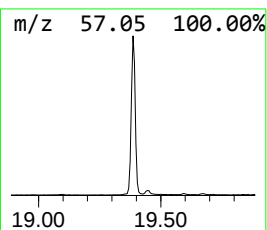
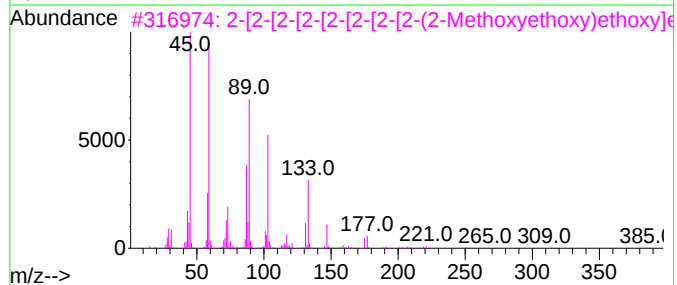
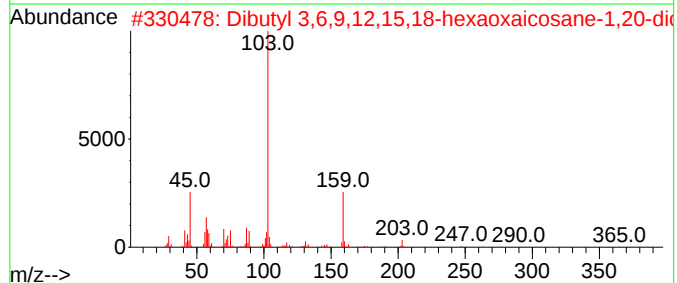
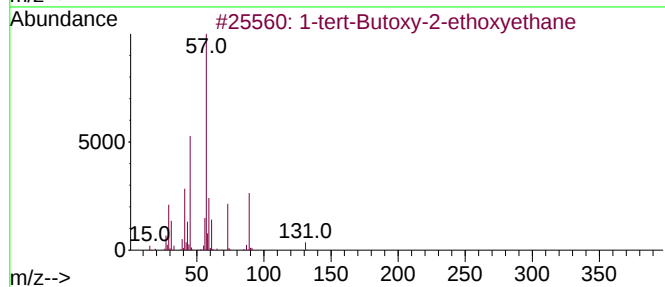
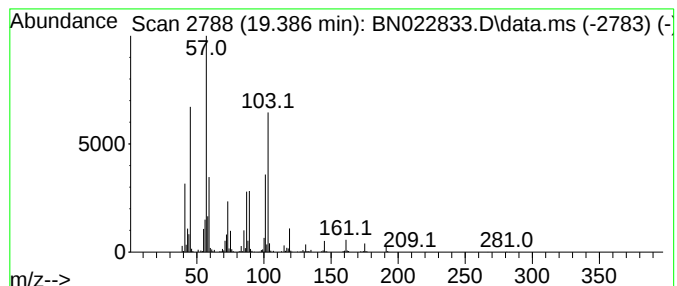
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.386	9.81 ng/ul	556260	Chrysene-d12	21.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	43		
2	Dibutyl 3,6,9,12,15,18-hexaoxaic...	466	C22H42O10	1000366-80-0	38		
3	2-[2-[2-[2-[2-[2-(2-Methox...	428	C19H40O10	006048-68-6	30		
4	2-[2-[2-[2-[2-[2-[2-[2-(2-...	516	C23H48O12	1010352-04-4	27		
5	2-[2-[2-[2-[2-[2-(2-Methoxyet...	384	C17H36O9	025990-96-9	27		



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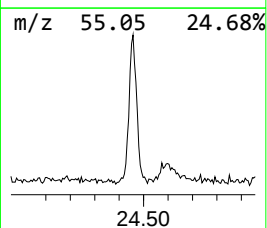
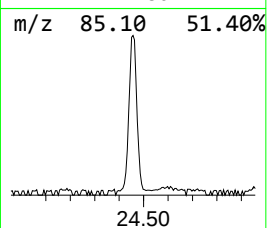
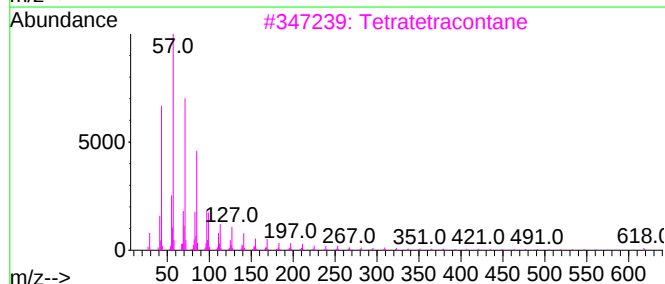
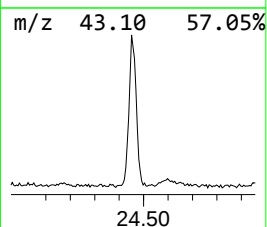
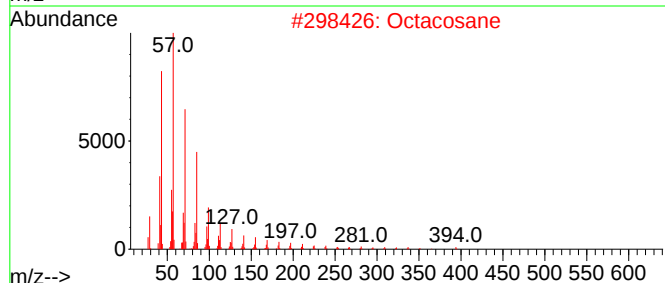
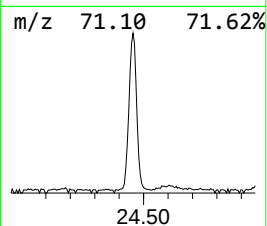
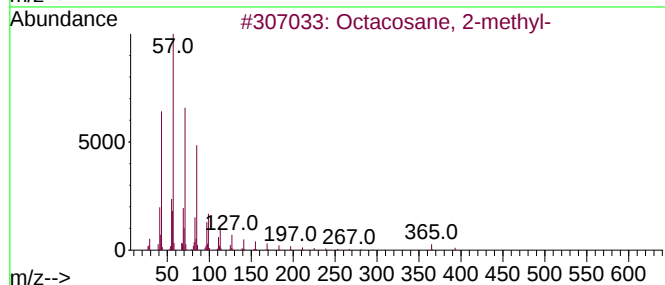
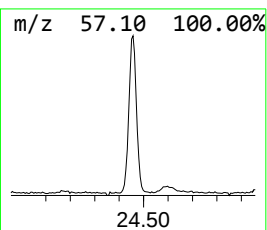
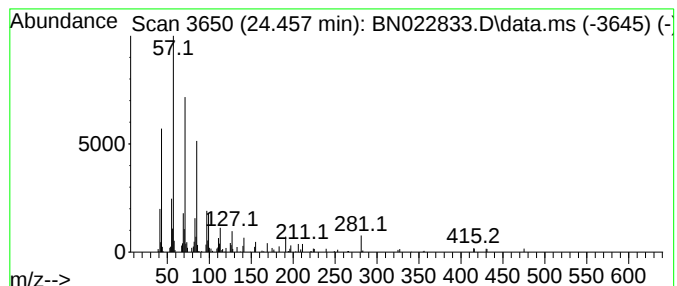
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.457	2.72 ng/ul	145291	Perylene-d12	23.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	81
2			Octacosane	394	C28H58	000630-02-4	81
3			Tetratetracontane	619	C44H90	007098-22-8	74
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	70
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	70



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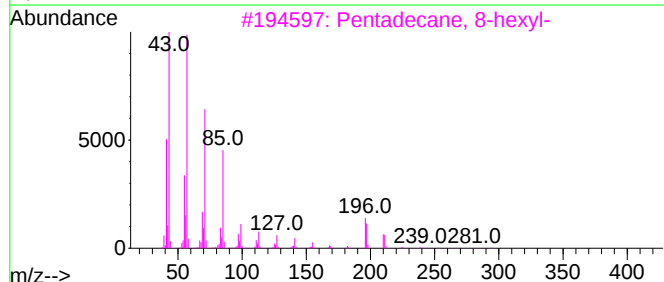
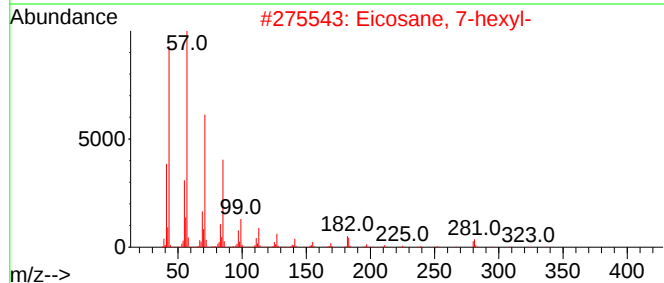
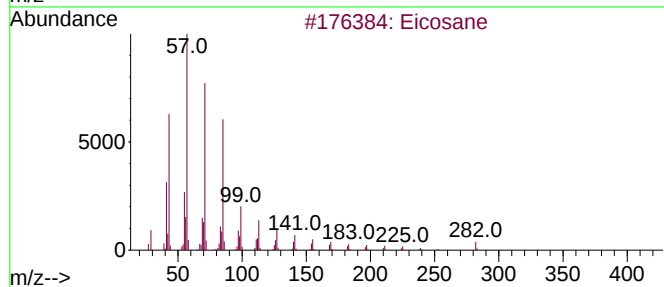
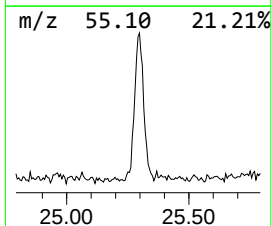
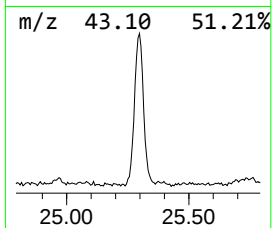
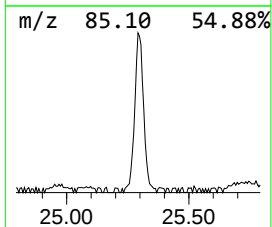
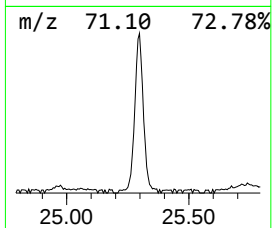
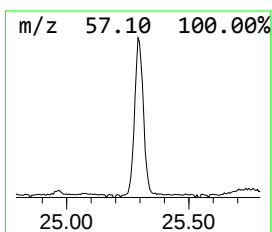
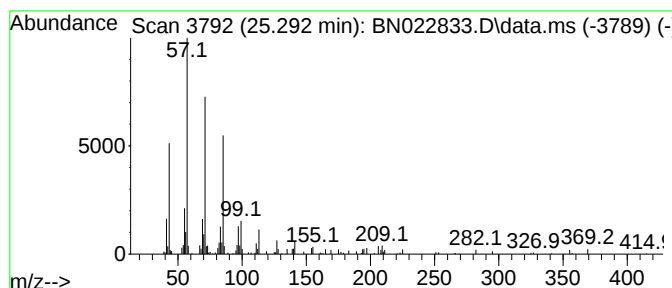
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.292	2.70 ng/ul	144602	Perylene-d12	23.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Eicosane	282	C20H42	000112-95-8	87
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86
4		Docosane, 11-butyl-	366	C26H54	013475-76-8	86
5		Tetracosane	338	C24H50	000646-31-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
Data File : BN022833.D
Acq On : 22 Nov 2022 20:21
Operator : CG/JU
Sample : N5593-10
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
H0AD9

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2(3H)-Benzothia...	16.216	2.1	ng/u1	110749	4	17.269	1036730	20.0
unknown-01	19.386	9.8	ng/u1	556260	5	21.469	1133870	20.0
(DEL) Alkane: S...	24.457	2.7	ng/u1	145291	6	23.863	1069290	20.0
(DEL) Alkane: S...	25.292	2.7	ng/u1	144602	6	23.863	1069290	20.0