

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
 Data File : BN033402.D
 Acq On : 15 Aug 2024 16:17
 Operator : MA/JU
 Sample : P3481-16
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 E0AF1

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-BN081424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN033402.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.158	25	29	38	rVB	72456	100238	1.29%	0.099%
2	3.411	68	72	89	rVB	189384	278110	3.58%	0.274%
3	3.546	90	95	109	rBV	644800	963929	12.40%	0.950%
4	3.728	122	126	131	rBV6	5521	8357	0.11%	0.008%
5	3.864	145	149	154	rVB	25012	32533	0.42%	0.032%
6	4.958	330	335	338	rBV	8896	14683	0.19%	0.014%
7	5.328	394	398	401	rBV4	6142	8854	0.11%	0.009%
8	5.693	456	460	466	rVB2	14334	22415	0.29%	0.022%
9	6.175	538	542	548	rBV5	7221	11426	0.15%	0.011%
10	6.569	606	609	618	rVB8	6608	14410	0.19%	0.014%
11	6.746	631	639	648	rBV	1402921	2197802	28.28%	2.166%
12	6.869	654	660	662	rBV	29754	42745	0.55%	0.042%
13	6.916	662	668	679	rVB	1190085	1783674	22.95%	1.758%
14	7.105	693	700	708	rBV	1466412	2214946	28.50%	2.183%
15	7.181	708	713	724	rVB	135607	211478	2.72%	0.208%
16	7.569	772	779	788	rVV	2229666	3409474	43.87%	3.361%
17	7.646	788	792	798	rVB2	14986	22034	0.28%	0.022%
18	7.869	827	830	835	rBV6	6314	12091	0.16%	0.012%
19	8.269	889	898	913	rBV	1807107	2839509	36.53%	2.799%
20	8.710	964	973	981	rBV	1310624	2146823	27.62%	2.116%
21	8.893	999	1004	1010	rVB6	12389	17093	0.22%	0.017%
22	9.187	1051	1054	1059	rVB2	8359	11525	0.15%	0.011%
23	9.287	1065	1071	1078	rBV	94455	140822	1.81%	0.139%
24	9.422	1085	1094	1108	rBV	1006326	1618497	20.82%	1.595%
25	9.552	1113	1116	1124	rVB9	5286	9180	0.12%	0.009%
26	9.663	1131	1135	1141	rBV6	8067	13584	0.17%	0.013%
27	9.840	1160	1165	1169	rBV5	8996	15340	0.20%	0.015%
28	9.957	1178	1185	1198	rVB	1762363	2804576	36.08%	2.764%
29	10.134	1211	1215	1220	rVB7	8726	16043	0.21%	0.016%
30	10.334	1241	1249	1260	rBV	3207212	5164656	66.45%	5.091%
31	10.469	1264	1272	1283	rBV	1021353	1663384	21.40%	1.640%
32	10.893	1339	1344	1351	rVB	65658	98100	1.26%	0.097%
33	11.081	1369	1376	1382	rBV	371776	609119	7.84%	0.600%
34	11.140	1382	1386	1394	rVB6	14654	28733	0.37%	0.028%
35	11.575	1453	1460	1465	rBV5	5635	9855	0.13%	0.010%
36	11.851	1501	1507	1513	rBV3	12089	22740	0.29%	0.022%

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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
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37	11.928	1513	1520	1528	rVB2	40183	68154	0.88%	0.067%
38	12.204	1563	1567	1574	rVB	11134	19067	0.25%	0.019%
39	12.569	1624	1629	1633	rBV2	9502	15755	0.20%	0.016%
40	12.710	1647	1653	1656	rBV7	5300	9240	0.12%	0.009%

41	12.822	1667	1672	1677	rBV4	11726	19980	0.26%	0.020%
42	13.063	1710	1713	1716	rVV5	6017	8791	0.11%	0.009%
43	13.192	1728	1735	1740	rVV9	9467	19645	0.25%	0.019%
44	13.428	1766	1775	1777	rBV6	6901	12330	0.16%	0.012%
45	13.628	1803	1809	1817	rBV	2969130	4030291	51.86%	3.973%

46	13.898	1847	1855	1862	rBV	3448943	5094501	65.55%	5.021%
47	14.210	1900	1908	1915	rBV	4720366	6767172	87.07%	6.670%
48	14.410	1932	1942	1946	rBV	1253116	1838082	23.65%	1.812%
49	14.445	1946	1948	1949	rVV2	31849	31471	0.40%	0.031%
50	14.563	1965	1968	1972	rVB6	5667	8532	0.11%	0.008%

51	14.657	1976	1984	1987	rBV4	24306	42948	0.55%	0.042%
52	14.739	1994	1998	2000	rBV4	6184	9567	0.12%	0.009%
53	15.045	2046	2050	2056	rBV2	16992	25363	0.33%	0.025%
54	15.104	2057	2060	2064	rVB3	8064	9394	0.12%	0.009%
55	15.204	2071	2077	2090	rVB	4174516	6075647	78.17%	5.989%

56	15.322	2090	2097	2109	rBV	912677	1249382	16.08%	1.231%
57	15.445	2114	2118	2123	rVB3	23772	34715	0.45%	0.034%
58	15.516	2128	2130	2134	rVB5	7587	8617	0.11%	0.008%
59	15.669	2152	2156	2160	rVB6	9275	11311	0.15%	0.011%
60	15.786	2171	2176	2183	rBV3	19792	32323	0.42%	0.032%

61	15.975	2204	2208	2209	rBV2	14022	17243	0.22%	0.017%
62	16.263	2254	2257	2260	rVB4	7432	8263	0.11%	0.008%
63	16.392	2275	2279	2284	rBV	58563	76383	0.98%	0.075%
64	16.551	2303	2306	2310	rVB5	8852	10996	0.14%	0.011%
65	16.710	2331	2333	2335	rBV3	7438	8300	0.11%	0.008%

66	16.739	2335	2338	2341	rBV	14463	20498	0.26%	0.020%
67	16.810	2347	2350	2353	rBV5	8128	12780	0.16%	0.013%
68	16.957	2367	2375	2381	rBV	5740562	7772139	100.00%	7.661%
69	16.998	2381	2382	2385	rVB	23409	16411	0.21%	0.016%
70	17.057	2385	2392	2404	rVB	4534120	6323085	81.36%	6.232%

71	17.163	2406	2410	2416	rBV3	61117	82720	1.06%	0.082%
72	17.222	2417	2420	2425	rBV2	16299	21920	0.28%	0.022%
73	17.269	2426	2428	2431	rBV	10512	10889	0.14%	0.011%
74	17.339	2435	2440	2451	rVV	306512	521323	6.71%	0.514%
75	17.669	2494	2496	2505	rVB	41443	56854	0.73%	0.056%

76	17.757	2507	2511	2519	rBV	98345	159691	2.05%	0.157%
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77	17.892	2528	2534	2542	rBV	1155281	1575474	20.27%	1.553%
78	18.180	2579	2583	2589	rVB6	33340	63659	0.82%	0.063%
79	18.333	2606	2609	2615	rVB6	27012	34319	0.44%	0.034%
80	18.563	2645	2648	2652	rBV5	16799	23111	0.30%	0.023%
81	18.763	2678	2682	2687	rBV6	32449	52849	0.68%	0.052%
82	18.851	2693	2697	2703	rVB5	59061	90926	1.17%	0.090%
83	18.922	2705	2709	2714	rVB	66698	82295	1.06%	0.081%
84	18.992	2717	2721	2723	rBV	83450	112459	1.45%	0.111%
85	19.027	2723	2727	2730	rVV2	121922	196053	2.52%	0.193%
86	19.057	2730	2732	2743	rVB2	126274	222640	2.86%	0.219%
87	19.186	2749	2754	2762	rBV	456073	690924	8.89%	0.681%
88	19.357	2777	2783	2789	rBV	5307934	7309672	94.05%	7.205%
89	19.422	2789	2794	2798	rVV	782239	1007349	12.96%	0.993%
90	19.963	2883	2886	2890	rBV	142248	155051	1.99%	0.153%
91	20.463	2968	2971	2975	rVB	180470	178211	2.29%	0.176%
92	20.927	3045	3050	3061	rBV3	455970	843898	10.86%	0.832%
93	21.192	3089	3095	3101	rBV2	4953510	6811802	87.64%	6.714%
94	21.439	3133	3137	3141	rVB	194036	234929	3.02%	0.232%
95	21.986	3226	3230	3237	rVB2	178841	271257	3.49%	0.267%
96	22.604	3331	3335	3343	rVB3	132532	231829	2.98%	0.229%
97	22.768	3358	3363	3369	rVB	342806	558696	7.19%	0.551%
98	23.315	3452	3456	3462	rVB2	101378	168912	2.17%	0.166%
99	23.827	3535	3543	3563	rVB	2361517	5399708	69.48%	5.322%
100	24.021	3567	3576	3590	rVB	2563944	5998074	77.17%	5.912%

Sum of corrected areas: 101454648

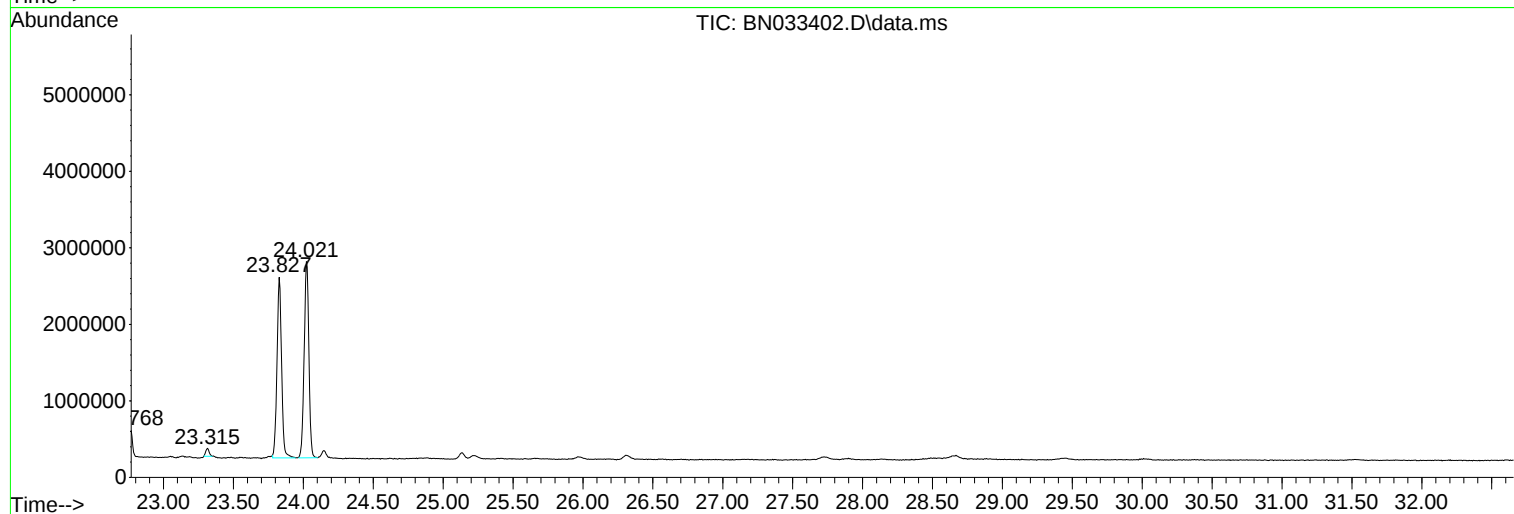
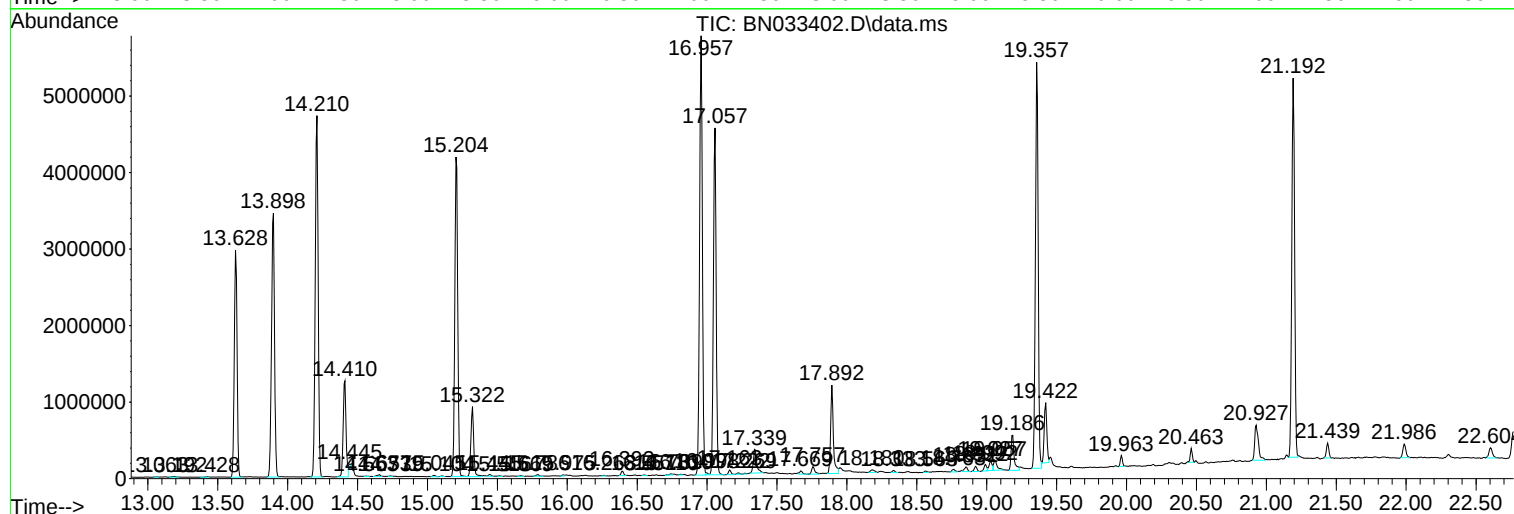
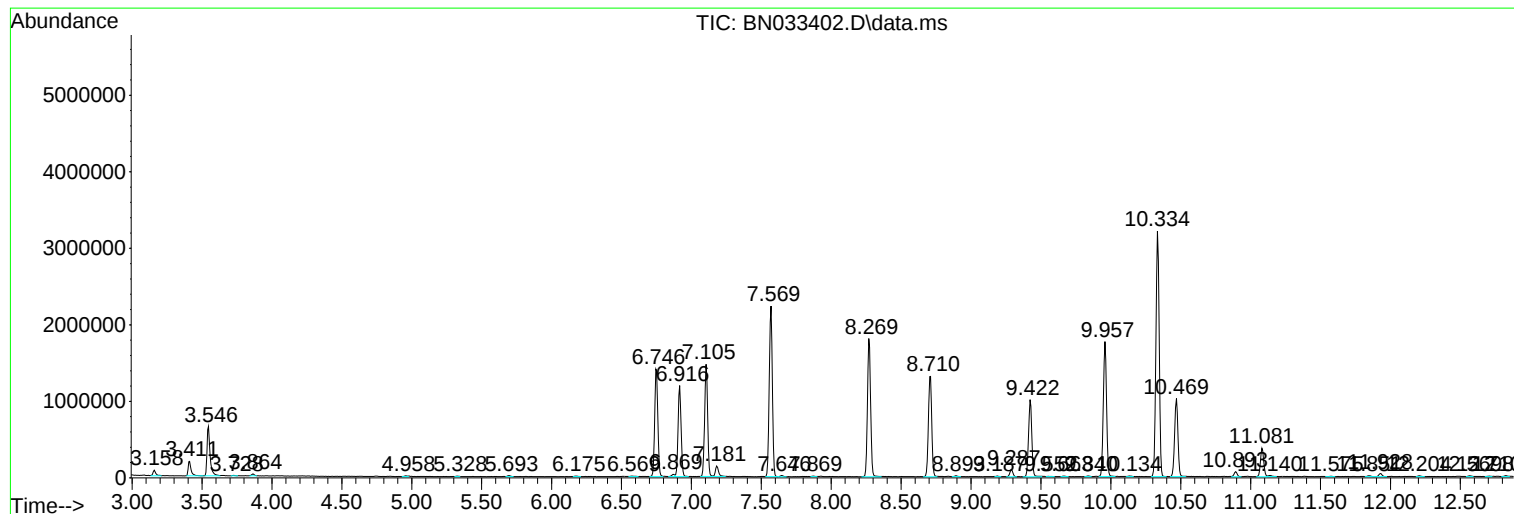
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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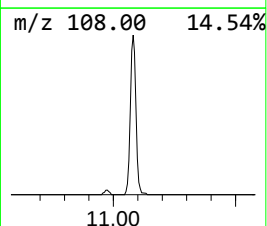
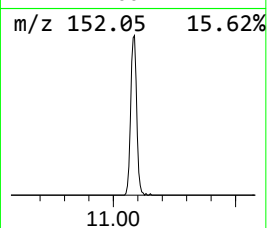
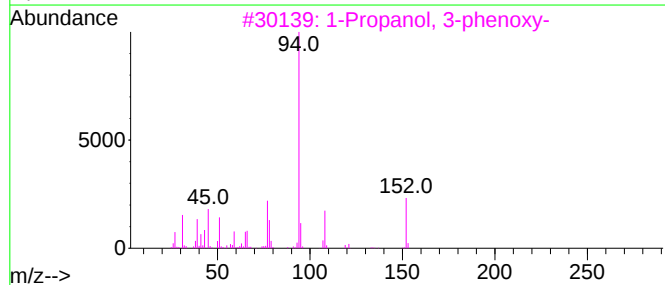
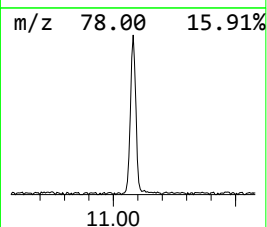
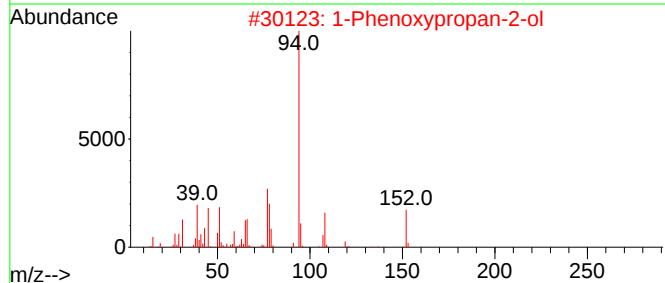
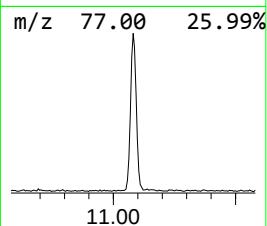
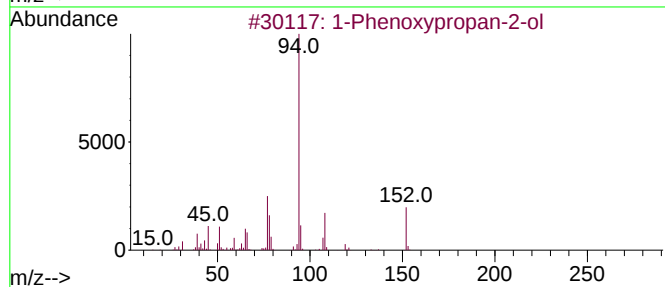
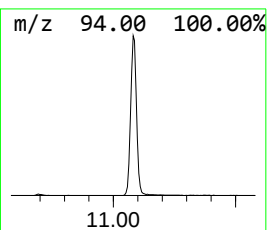
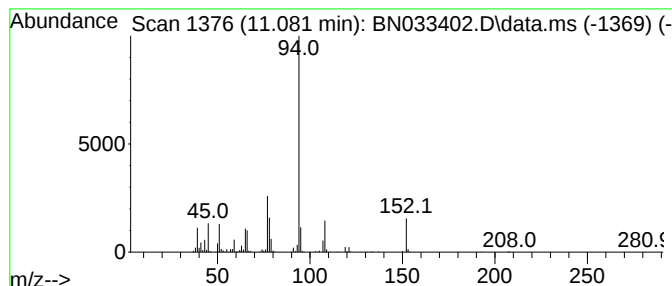
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.081	2.36 ng/ul	609119	Naphthalene-d8	10.334

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	91
5			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87



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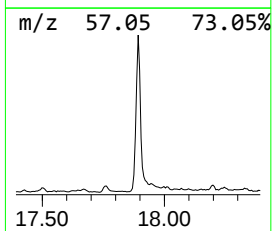
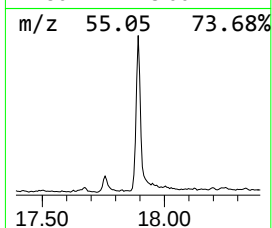
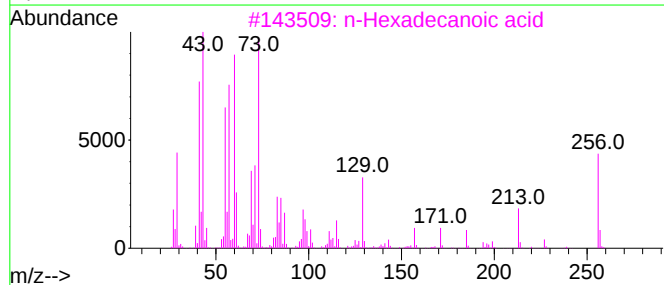
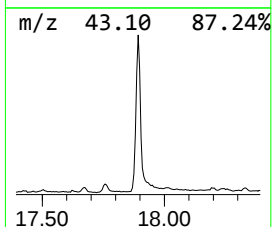
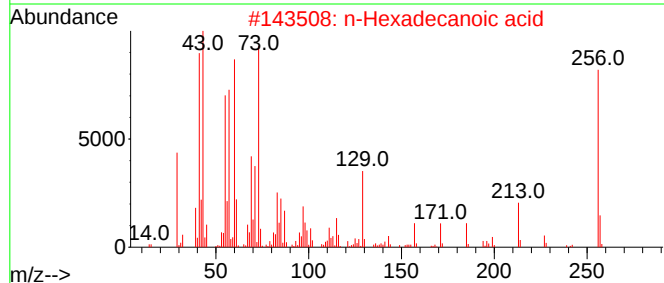
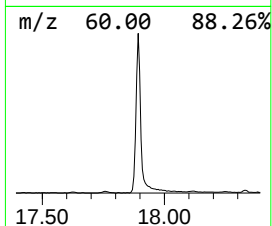
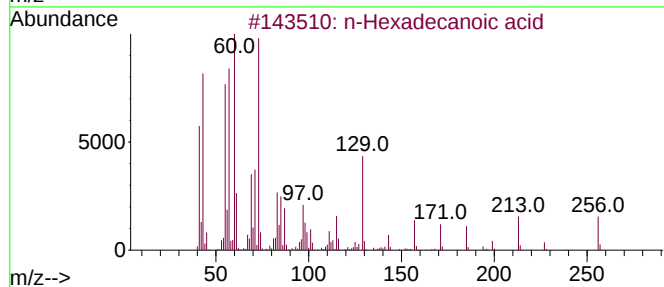
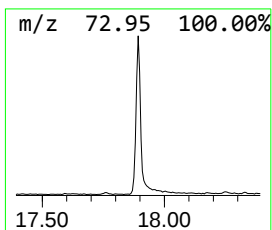
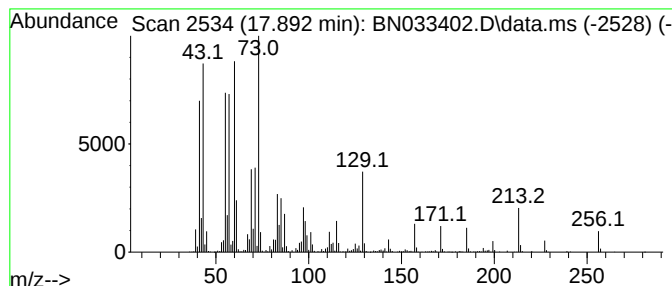
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.892	4.05 ng/ul	1575470	Phenanthrene-d10	16.957

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	99		
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98		
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97		
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93		



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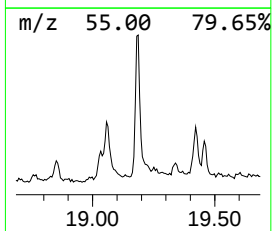
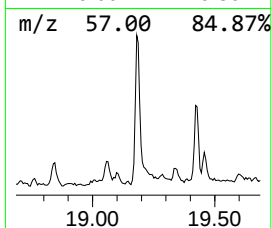
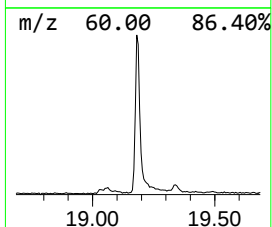
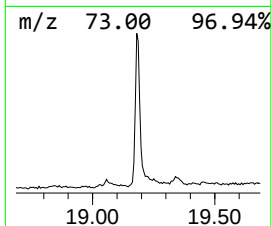
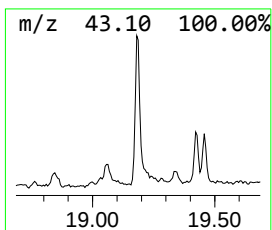
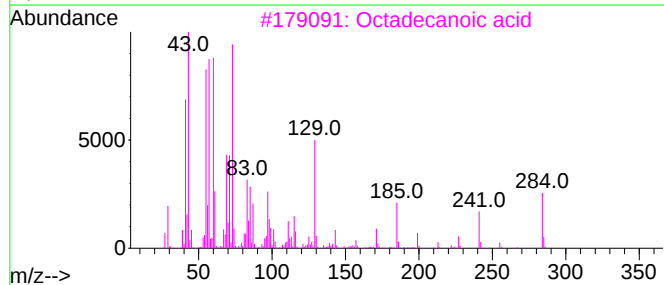
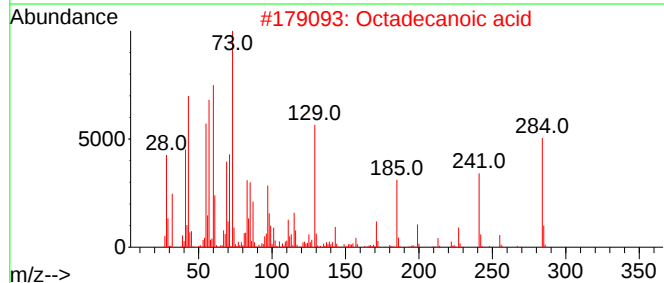
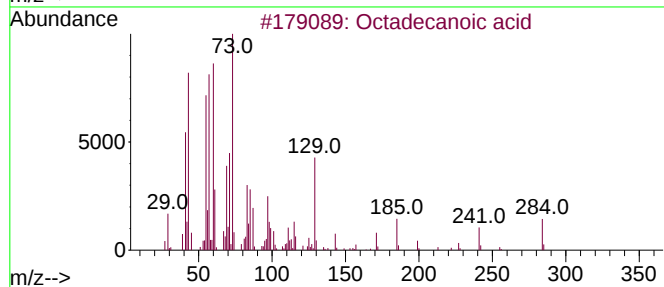
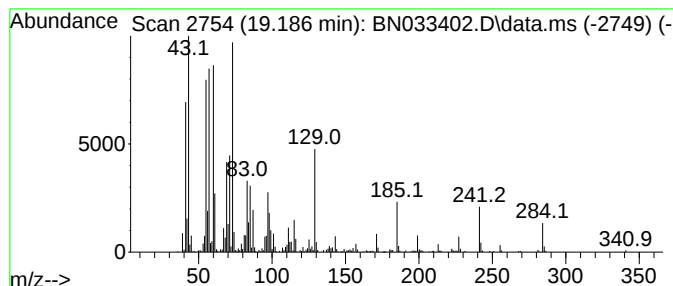
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.186	2.03 ng/ul	690924	Chrysene-d12	21.192

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	99
3	Octadecanoic acid			284	C18H36O2	000057-11-4	99
4	Octadecanoic acid			284	C18H36O2	000057-11-4	96
5	Octadecanoic acid			284	C18H36O2	000057-11-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033402.D
Acq On : 15 Aug 2024 16:17
Operator : MA/JU
Sample : P3481-16
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AF1

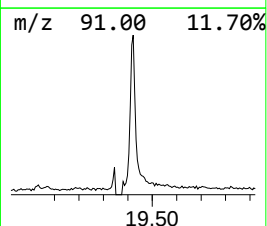
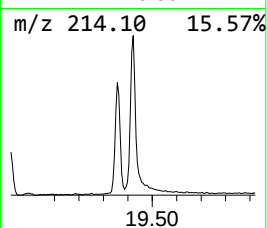
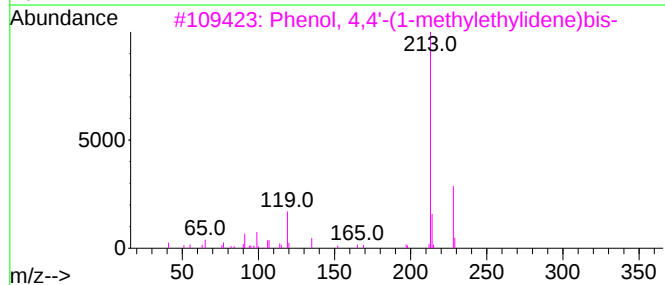
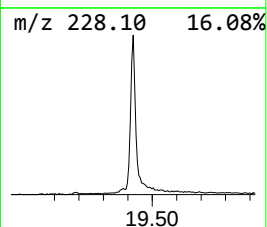
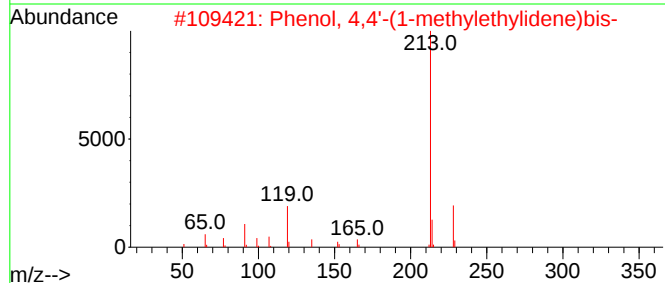
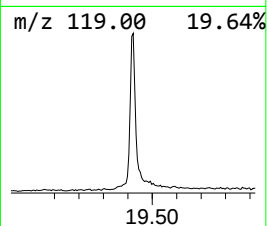
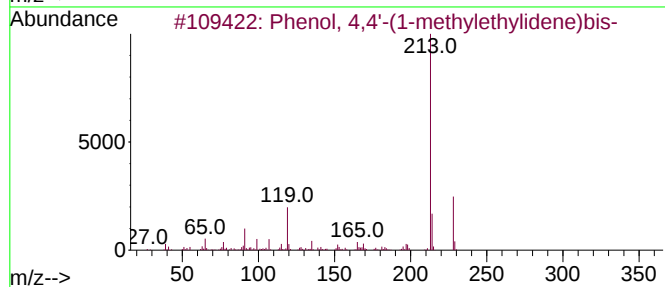
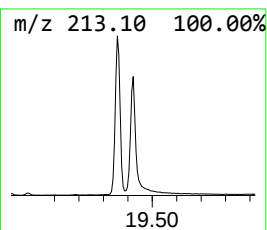
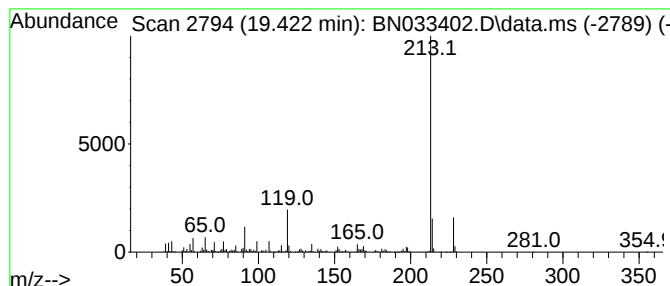
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	2.96 ng/ul	1007350	Chrysene-d12	21.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	95
3			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	90
4			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	87
5			Diphenolic acid	286	C17H18O4	000126-00-1	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033402.D
Acq On : 15 Aug 2024 16:17
Operator : MA/JU
Sample : P3481-16
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AF1

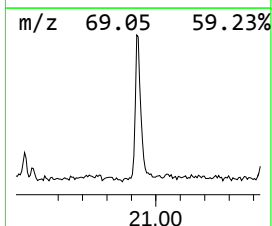
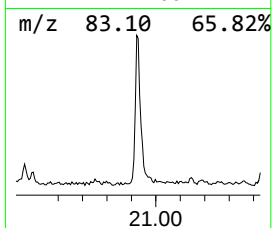
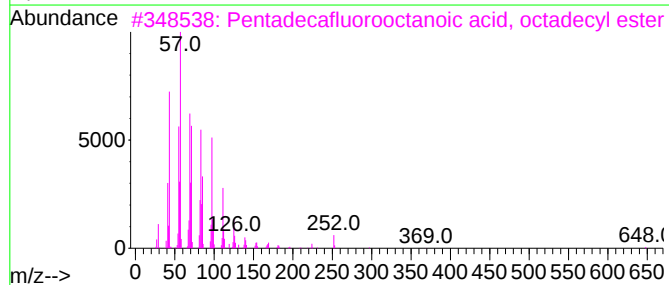
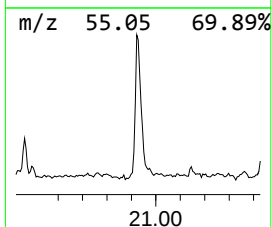
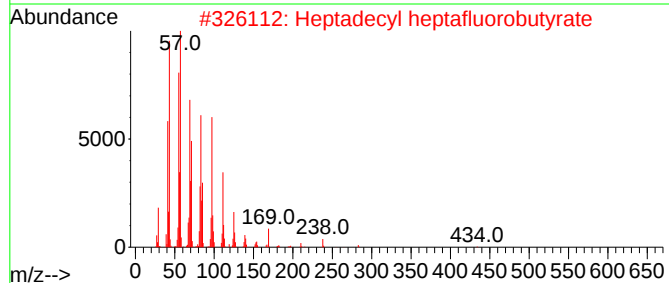
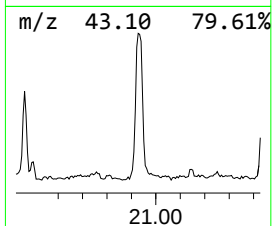
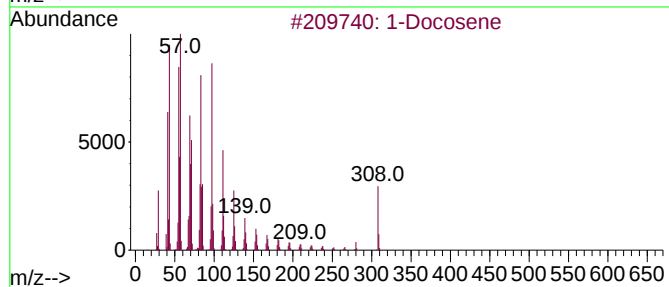
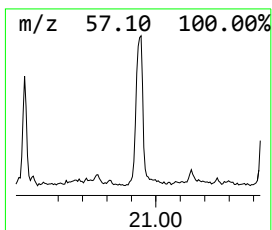
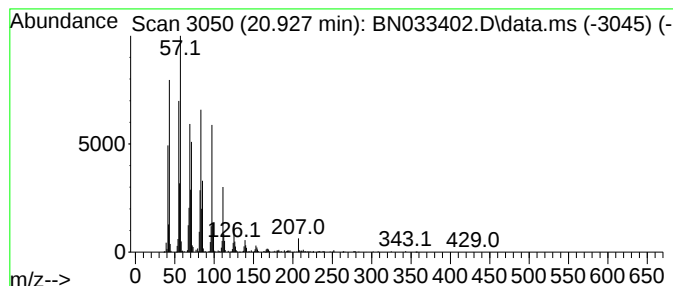
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.927	2.48 ng/ul	843898	Chrysene-d12	21.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	97
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	94
4	Heptafluorobutyric acid, n-octad...			466	C22H37F7O2	000400-57-7	94
5	1-Hexacosene			364	C26H52	018835-33-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN081524\
Data File : BN033402.D
Acq On : 15 Aug 2024 16:17
Operator : MA/JU
Sample : P3481-16
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
E0AF1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN081424.MA.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
1-Phenoxypropan...	11.081	2.4	ng/ul	609119	2	10.334	5164660	20.0
n-Hexadecanoic ...	17.892	4.0	ng/ul	1575470	4	16.957	7772140	20.0
Octadecanoic acid	19.186	2.0	ng/ul	690924	5	21.192	6811800	20.0
Phenol, 4,4'-(1...	19.422	3.0	ng/ul	1007350	5	21.192	6811800	20.0
(DEL) Alkane: S...	20.927	2.5	ng/ul	843898	5	21.192	6811800	20.0