

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120822\
 Data File : BP012992.D
 Acq On : 08 Dec 2022 19:23
 Operator : CG/JU
 Sample : N5894-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AA6

Integration Parameters: LSCINT.P

Integrator: RTE

Soothing : 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-BP120722.M
 Title : SVOA CALIBRATION

Signal : TIC: BP012992.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.352	24	28	37	rBV	118428	179374	1.01%	0.109%
2	3.787	99	102	116	rBV	319494	583506	3.27%	0.354%
3	3.976	130	134	137	rBV	23280	34118	0.19%	0.021%
4	4.017	137	141	147	rVB2	66327	114647	0.64%	0.069%
5	4.117	154	158	162	rVB	43686	61882	0.35%	0.037%
6	4.493	218	222	229	rVB7	19830	35454	0.20%	0.021%
7	5.064	314	319	325	rBV4	17399	30698	0.17%	0.019%
8	5.452	378	385	390	rVV6	15787	29982	0.17%	0.018%
9	5.593	404	409	412	rBV6	10053	18369	0.10%	0.011%
10	5.799	441	444	448	rBV5	11122	18182	0.10%	0.011%
11	5.881	455	458	463	rBV2	15785	22969	0.13%	0.014%
12	5.964	469	472	477	rVB4	13082	21139	0.12%	0.013%
13	6.870	622	626	632	rVB7	12422	20743	0.12%	0.013%
14	6.946	634	639	645	rBV2	38601	69042	0.39%	0.042%
15	7.128	664	670	680	rVB	538625	845836	4.74%	0.512%
16	7.299	692	699	708	rBV	1945318	2996351	16.81%	1.815%
17	7.505	724	734	743	rVV	1820924	2919284	16.37%	1.769%
18	7.593	745	749	757	rVB7	19838	34205	0.19%	0.021%
19	7.975	806	814	819	rBV	1991129	3135257	17.59%	1.900%
20	8.034	819	824	834	rVB	828113	1300710	7.30%	0.788%
21	8.211	848	854	856	rBV6	21886	37343	0.21%	0.023%
22	8.246	857	860	867	rVB	35919	55627	0.31%	0.034%
23	8.528	902	908	915	rBV7	25260	56501	0.32%	0.034%
24	8.681	923	934	942	rBV	1607485	2560169	14.36%	1.551%
25	9.140	1005	1012	1021	rVV	2295421	3613919	20.27%	2.190%
26	9.252	1021	1031	1036	rVV2	112984	251693	1.41%	0.152%
27	9.299	1036	1039	1046	rVB7	20071	32776	0.18%	0.020%
28	9.552	1076	1082	1088	rVB8	18818	37932	0.21%	0.023%
29	9.869	1127	1136	1147	rBV	1732872	2874210	16.12%	1.741%
30	10.022	1153	1162	1168	rBV	170091	362370	2.03%	0.220%
31	10.093	1168	1174	1187	rVB	138571	257260	1.44%	0.156%
32	10.405	1220	1227	1237	rBV	2849674	4710510	26.42%	2.854%
33	10.563	1248	1254	1261	rBV	117981	196391	1.10%	0.119%
34	10.787	1285	1292	1300	rBV	2855619	4794596	26.89%	2.905%
35	10.922	1309	1315	1333	rBV	1239467	2209340	12.39%	1.339%
36	11.446	1396	1404	1412	rBV	125633	231477	1.30%	0.140%

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Integrator: RTE

Smoothing : OFF

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
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37	11.581	1418	1427	1437	rBV	329332	583579	3.27%	0.354%
38	11.758	1454	1457	1462	rVB2	20511	28900	0.16%	0.018%
39	12.116	1511	1518	1526	rBV2	10539	20485	0.11%	0.012%
40	12.275	1539	1545	1552	rBV4	15918	29487	0.17%	0.018%
41	12.369	1552	1561	1568	rBV2	63353	110330	0.62%	0.067%
42	12.881	1642	1648	1655	rBV	68603	119497	0.67%	0.072%
43	13.046	1671	1676	1680	rBV8	9579	21252	0.12%	0.013%
44	13.240	1703	1709	1713	rVB4	15235	28381	0.16%	0.017%
45	13.440	1737	1743	1745	rBV4	15512	29661	0.17%	0.018%
46	13.504	1749	1754	1758	rBV3	38623	65513	0.37%	0.040%
47	13.587	1763	1768	1773	rVV7	23605	41440	0.23%	0.025%
48	14.022	1835	1842	1848	rBV	5945049	8320363	46.67%	5.041%
49	14.134	1857	1861	1868	rVB7	27691	56019	0.31%	0.034%
50	14.263	1878	1883	1885	rBV	215296	285741	1.60%	0.173%
51	14.310	1885	1891	1901	rVV	6530433	9619801	53.96%	5.829%
52	14.393	1901	1905	1911	rVB	190131	260098	1.46%	0.158%
53	14.499	1921	1923	1927	rVB3	19376	24098	0.14%	0.015%
54	14.616	1932	1943	1952	rBV	4570242	6897789	38.69%	4.179%
55	14.799	1969	1974	1981	rBV	411354	669923	3.76%	0.406%
56	14.893	1986	1990	1994	rVB6	19493	29399	0.16%	0.018%
57	14.957	1995	2001	2005	rBV8	24445	50335	0.28%	0.030%
58	15.016	2006	2011	2016	rVB2	95952	148951	0.84%	0.090%
59	15.122	2025	2029	2034	rVB6	20006	37821	0.21%	0.023%
60	15.310	2056	2061	2066	rBV5	20226	40749	0.23%	0.025%
61	15.404	2073	2077	2080	rBV	36413	54581	0.31%	0.033%
62	15.475	2085	2089	2093	rVB2	78420	110186	0.62%	0.067%
63	15.604	2104	2111	2123	rBV	8535523	12840441	72.02%	7.780%
64	15.722	2124	2131	2145	rVB	2634551	3698636	20.74%	2.241%
65	15.846	2148	2152	2158	rVV5	60469	122813	0.69%	0.074%
66	15.910	2158	2163	2168	rVV9	19723	37171	0.21%	0.023%
67	16.246	2217	2220	2223	rBV	49283	60114	0.34%	0.036%
68	16.287	2223	2227	2230	rVV2	34900	56298	0.32%	0.034%
69	16.316	2230	2232	2236	rVB4	24315	26386	0.15%	0.016%
70	16.451	2253	2255	2259	rVB3	30314	33477	0.19%	0.020%
71	16.604	2278	2281	2288	rBV8	29418	46886	0.26%	0.028%
72	16.681	2288	2294	2299	rVV3	72195	125110	0.70%	0.076%
73	16.751	2302	2306	2314	rVV	213739	297768	1.67%	0.180%
74	16.834	2316	2320	2327	rVB6	41364	70749	0.40%	0.043%
75	17.116	2365	2368	2371	rBV4	19011	21107	0.12%	0.013%
76	17.275	2392	2395	2398	rVB4	31302	36841	0.21%	0.022%

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77	17.369	2405	2411	2418	rBV	6090657	8474222	47.53%	5.134%
78	17.469	2421	2428	2440	rVV	10187816	14373771	80.62%	8.709%
79	17.551	2440	2442	2450	rVB3	41125	51245	0.29%	0.031%
80	17.616	2450	2453	2456	rBV	60235	82763	0.46%	0.050%
81	17.645	2456	2458	2461	rVB	24245	26504	0.15%	0.016%
82	17.904	2499	2502	2505	rBV4	20293	27978	0.16%	0.017%
83	18.028	2519	2523	2527	rVB4	108863	134821	0.76%	0.082%
84	18.069	2527	2530	2533	rBV4	37224	55433	0.31%	0.034%
85	18.128	2533	2540	2549	rVV2	185472	373634	2.10%	0.226%
86	18.234	2554	2558	2565	rVV3	186428	290807	1.63%	0.176%
87	18.316	2568	2572	2580	rVB	80530	128754	0.72%	0.078%
88	18.445	2590	2594	2601	rVB2	77601	104736	0.59%	0.063%
89	19.063	2696	2699	2702	rBV2	49497	55740	0.31%	0.034%
90	19.275	2731	2735	2739	rVB	143658	173877	0.98%	0.105%
91	19.345	2742	2747	2756	rVV	166882	381125	2.14%	0.231%
92	19.463	2764	2767	2772	rVB3	135530	158920	0.89%	0.096%
93	19.539	2778	2780	2785	rVB3	81711	85568	0.48%	0.052%
94	19.698	2801	2807	2822	rBV	13519697	17623374	98.85%	10.678%
95	20.434	2928	2932	2943	rBV4	732903	1300583	7.29%	0.788%
96	20.539	2944	2950	2963	rVV	2762133	4335409	24.32%	2.627%
97	21.145	3050	3053	3057	rBV	249963	314710	1.77%	0.191%
98	21.451	3100	3105	3113	rBV	6838671	9322703	52.29%	5.649%
99	23.780	3494	3501	3518	rVB2	8177826	17829134	100.00%	10.803%
100	23.945	3522	3529	3540	rVB2	4592268	9428146	52.88%	5.712%

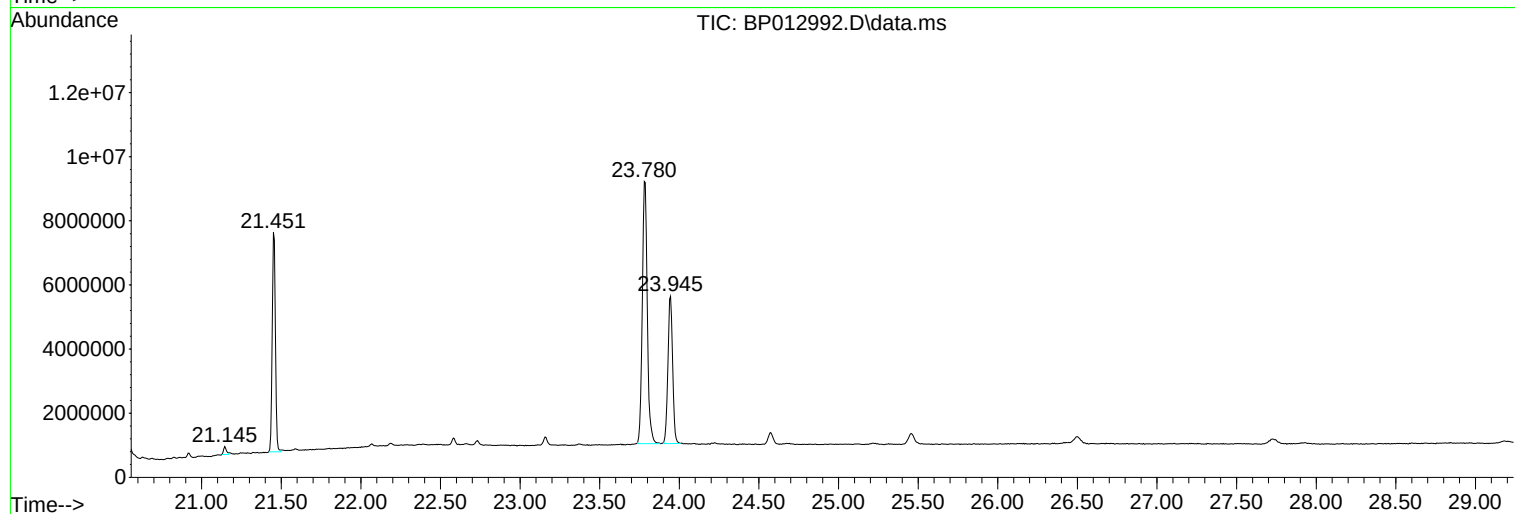
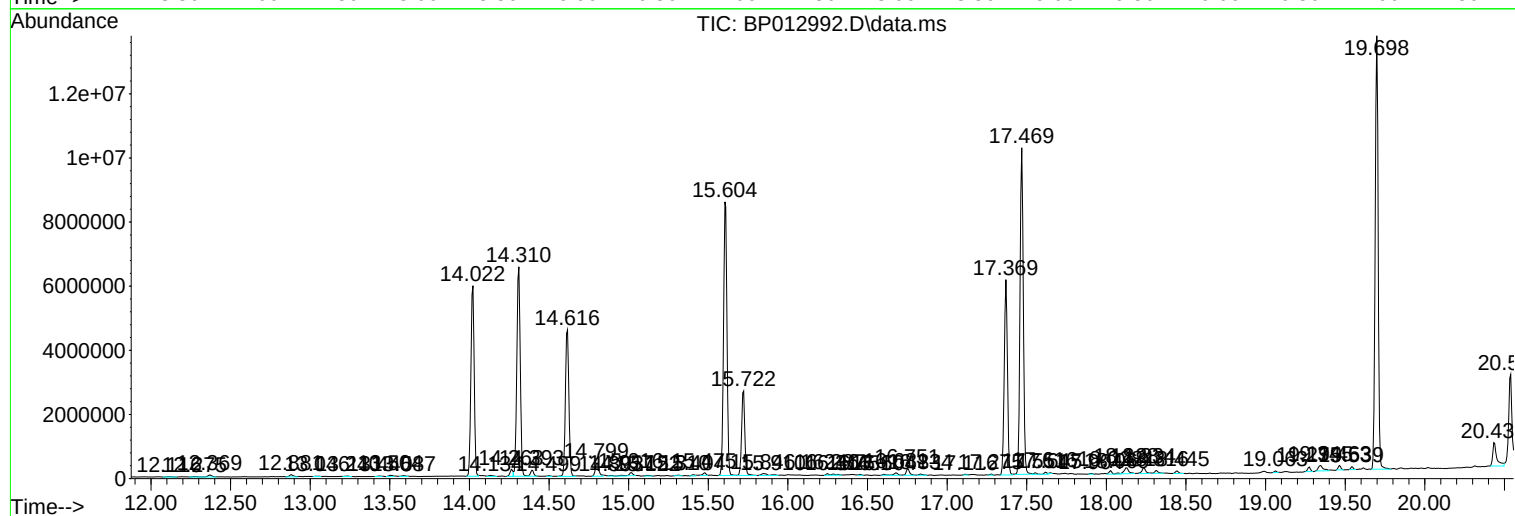
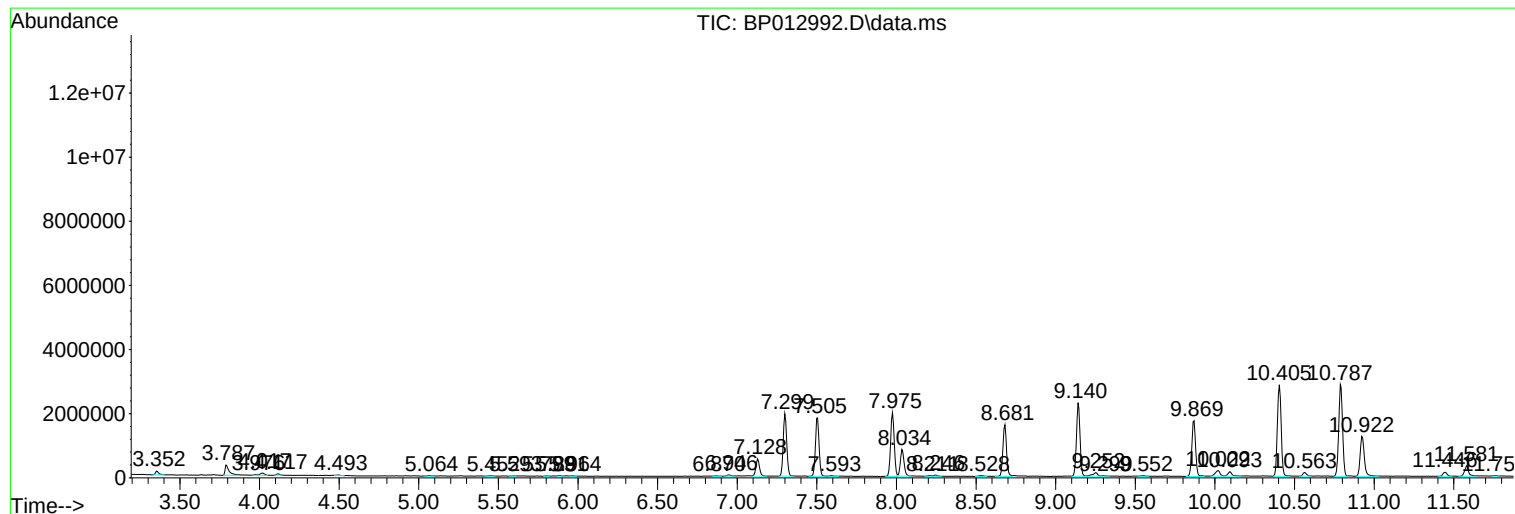
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



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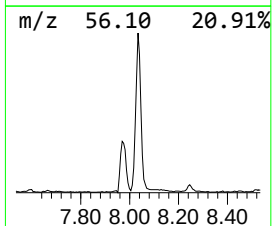
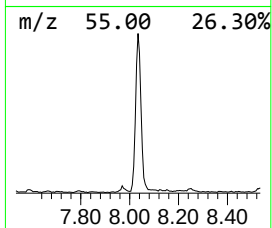
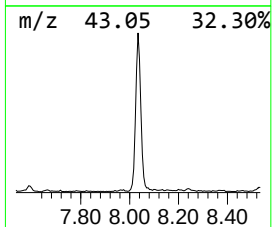
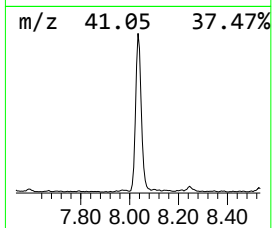
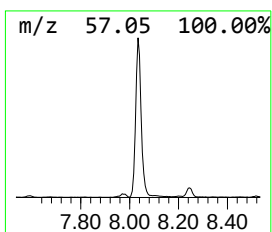
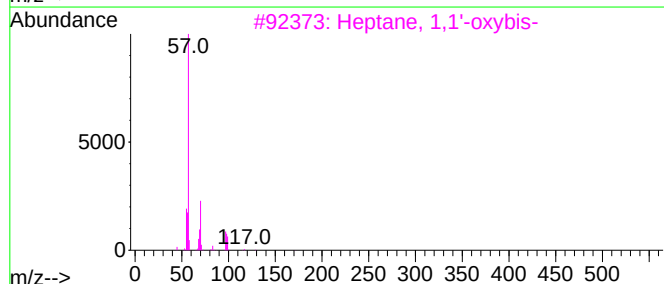
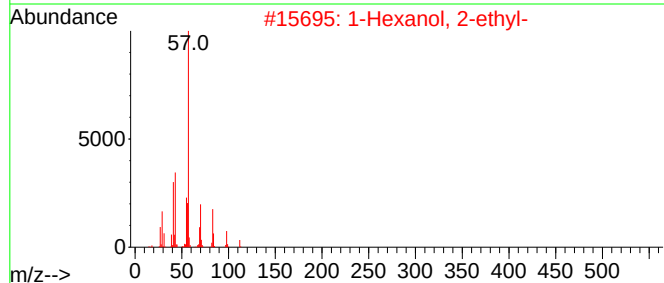
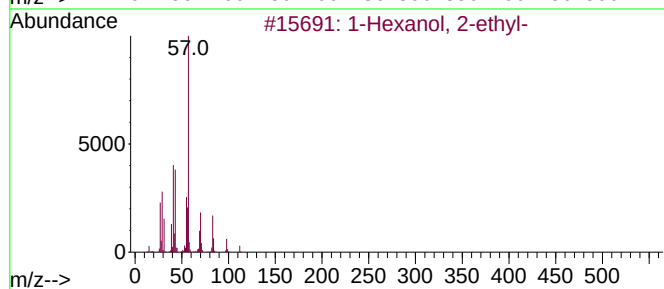
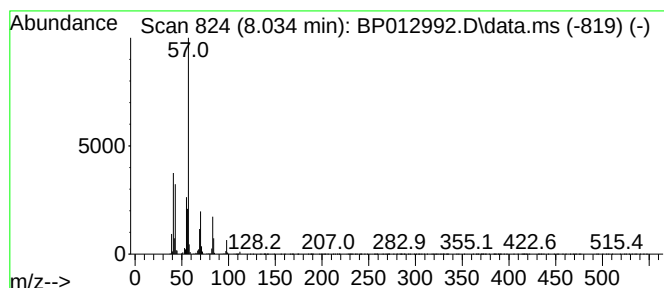
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.034	8.30 ng/ul	1300710	1,4-Dichlorobenzene-d4	7.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	Heptane, 1,1'-oxybis-			214	C14H30O	000629-64-1	64
4	1-Isobutoxy-2-ethylhexane			186	C12H26O	1000139-90-3	64
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64



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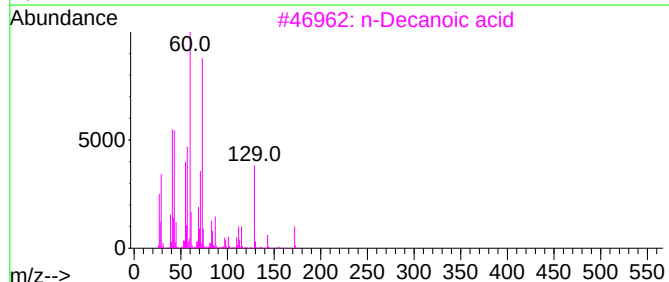
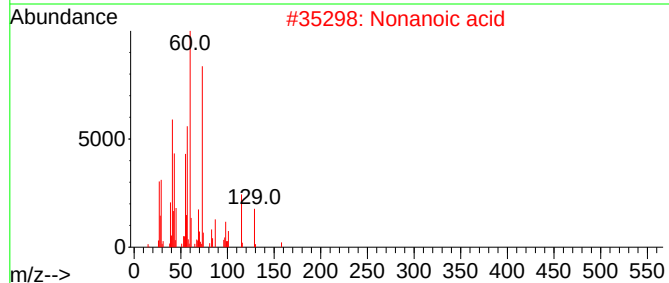
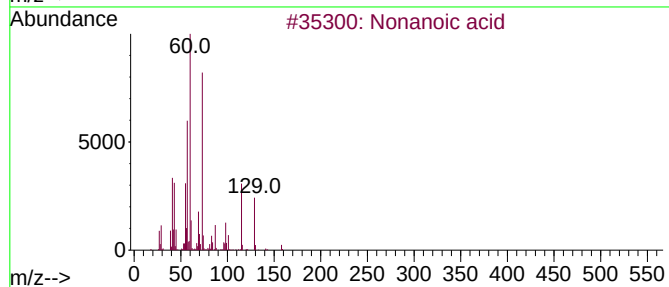
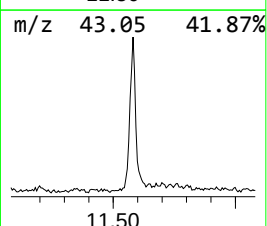
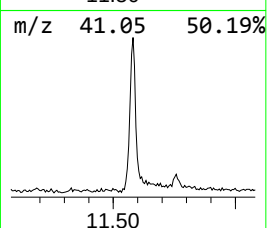
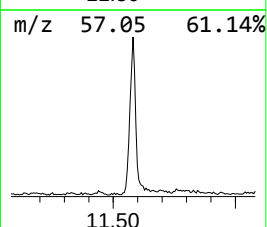
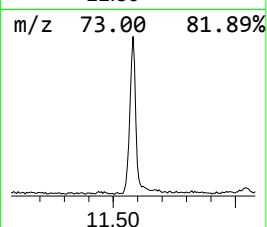
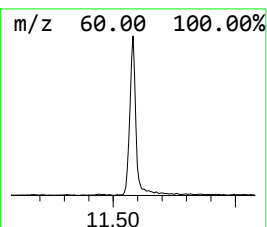
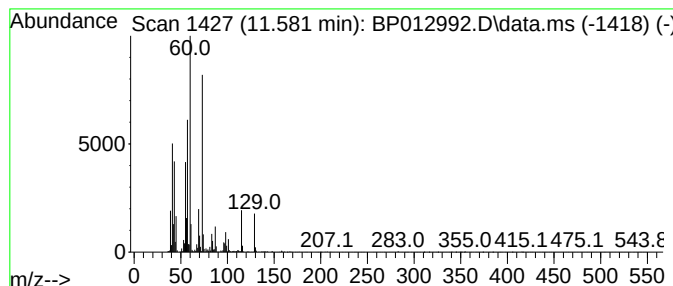
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Nonanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.581	2.43 ng/ul	583579	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	97
2			Nonanoic acid	158	C9H18O2	000112-05-0	91
3			n-Decanoic acid	172	C10H20O2	000334-48-5	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Nonanoic acid	158	C9H18O2	000112-05-0	64



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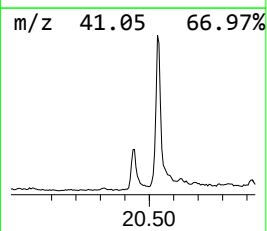
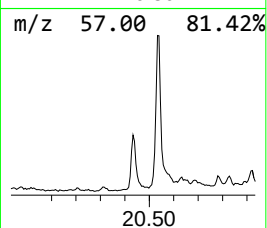
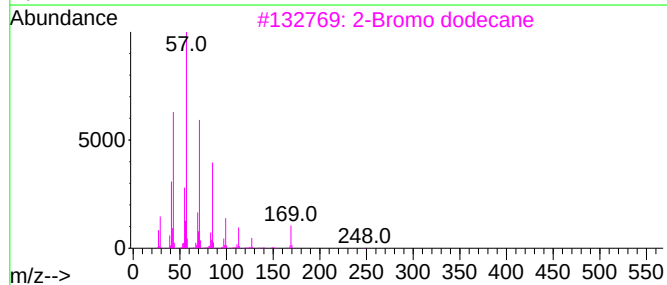
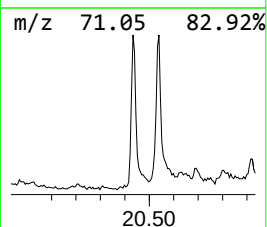
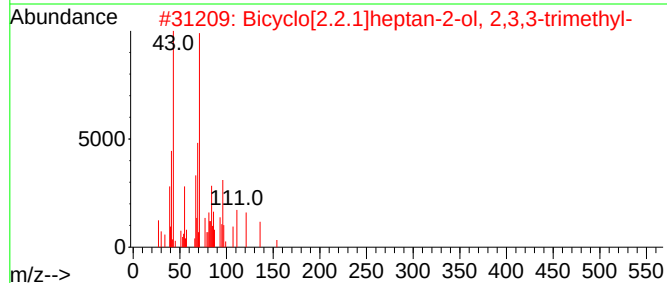
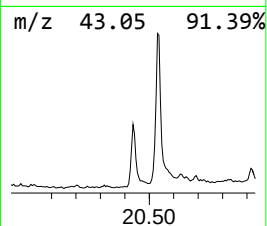
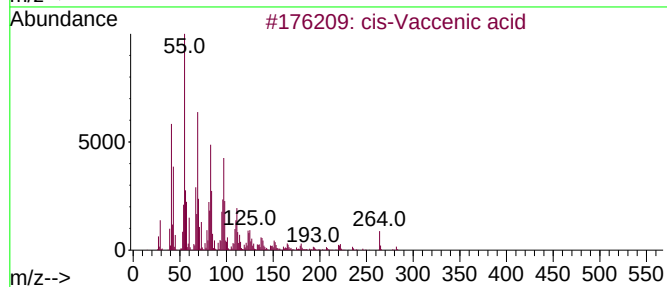
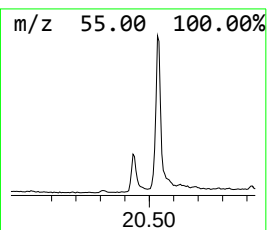
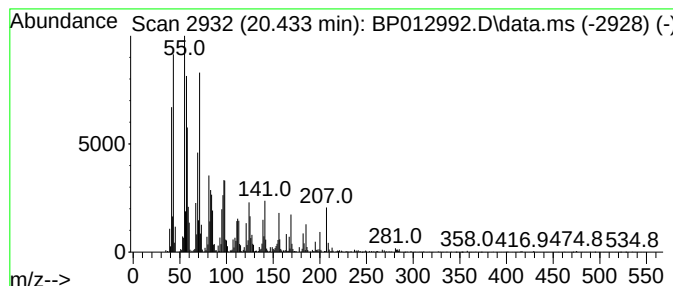
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.433	2.79 ng/ul	1300580	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	45
2			Bicyclo[2.2.1]heptan-2-ol, 2,3,3...	154	C10H18O	000465-31-6	41
3			2-Bromo dodecane	248	C12H25Br	013187-99-0	38
4			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	30
5			Octane, 4-ethyl-	142	C10H22	015869-86-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120822\
Data File : BP012992.D
Acq On : 08 Dec 2022 19:23
Operator : CG/JU
Sample : N5894-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AA6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

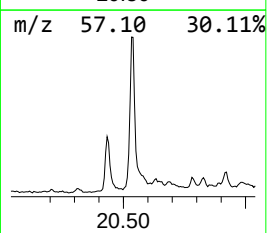
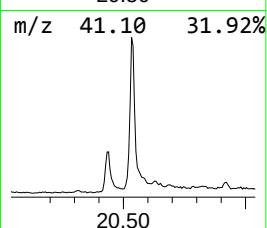
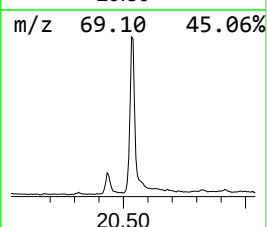
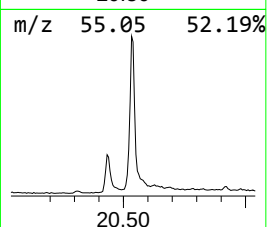
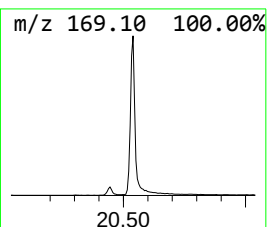
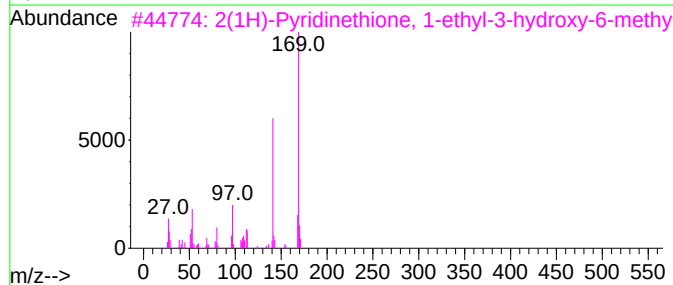
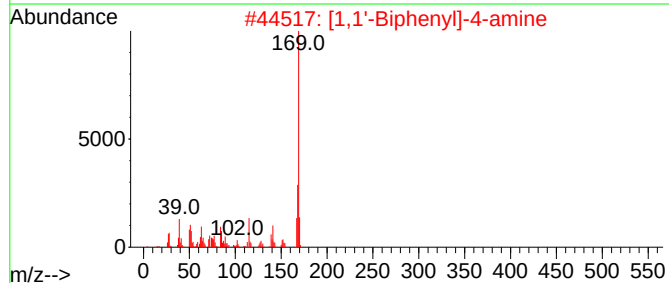
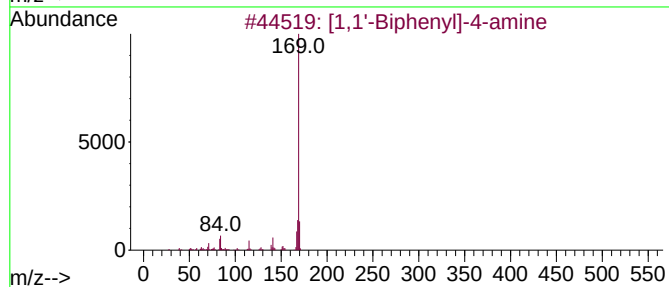
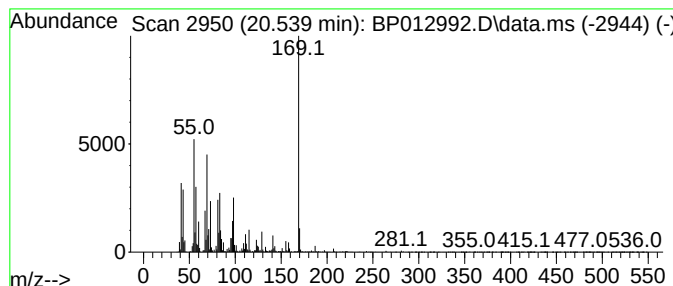
TIC Library : C:\DATABASE\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.539	9.30 ng/ul	4335410	Chrysene-d12	21.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			[1,1'-Biphenyl]-4-amine	169	C12H11N	000092-67-1	38
2			[1,1'-Biphenyl]-4-amine	169	C12H11N	000092-67-1	35
3			2(1H)-Pyridinethione, 1-ethyl-3-...	169	C8H11NOS	024207-15-6	35
4			3-Nitrothioanisole	169	C7H7NO2S	002524-76-7	35
5			[1,1'-Biphenyl]-3-amine	169	C12H11N	002243-47-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120822\
Data File : BP012992.D
Acq On : 08 Dec 2022 19:23
Operator : CG/JU
Sample : N5894-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AA6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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-Hexanol, 2-et...	8.034	8.3	ng/ul	1300710	1	7.975	3135260	20.0
Nonanoic acid	11.581	2.4	ng/ul	583579	2	10.787	4794600	20.0
unknown-01	20.433	2.8	ng/ul	1300580	5	21.451	9322700	20.0
unknown-02	20.539	9.3	ng/ul	4335410	5	21.451	9322700	20.0