

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
 Data File : BN029565.D
 Acq On : 08 Feb 2024 03:06
 Operator : MA/JU
 Sample : P1303-20
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 C0FJ7

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-BN020724.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN029565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.293	32	35	38	rBV3	11682	18506	0.34%	0.030%
2	3.328	38	41	47	rVB	81994	107343	1.99%	0.175%
3	3.740	107	111	119	rBV	410173	656050	12.17%	1.071%
4	3.805	119	122	127	rVV	91698	128384	2.38%	0.210%
5	3.858	127	131	136	rVB	41699	54913	1.02%	0.090%
6	3.970	147	150	156	rVB5	15579	23505	0.44%	0.038%
7	4.058	161	165	174	rVB2	35743	63365	1.18%	0.103%
8	4.293	201	205	211	rVB	23301	30764	0.57%	0.050%
9	4.399	218	223	227	rBV	127520	174724	3.24%	0.285%
10	4.440	227	230	236	rVB4	25058	38720	0.72%	0.063%
11	4.628	257	262	267	rBV	75592	107663	2.00%	0.176%
12	4.675	267	270	273	rBV	28617	37484	0.70%	0.061%
13	4.781	285	288	290	rBV4	5290	7322	0.14%	0.012%
14	4.999	317	325	337	rBV2	304561	492675	9.14%	0.804%
15	5.093	337	341	347	rVB5	9025	19947	0.37%	0.033%
16	5.617	427	430	436	rVB2	8592	13468	0.25%	0.022%
17	5.781	454	458	463	rVB7	7322	11611	0.22%	0.019%
18	6.199	526	529	537	rVB10	6980	13923	0.26%	0.023%
19	6.869	638	643	647	rBV8	4956	9213	0.17%	0.015%
20	7.052	666	674	689	rBV	1243647	2037387	37.78%	3.326%
21	7.228	697	704	713	rBV	1047563	1600444	29.68%	2.613%
22	7.411	728	735	747	rBV	1229036	1933475	35.85%	3.156%
23	7.581	760	764	771	rVB8	11596	20797	0.39%	0.034%
24	7.887	809	816	823	rBV	854810	1374494	25.49%	2.244%
25	7.952	823	827	832	rVB2	14430	21353	0.40%	0.035%
26	8.046	839	843	846	rBV5	6263	8401	0.16%	0.014%
27	8.134	852	858	859	rBV6	9098	14025	0.26%	0.023%
28	8.593	929	936	951	rBV	1178578	1881104	34.88%	3.071%
29	8.716	951	957	965	rVB	97663	159451	2.96%	0.260%
30	9.052	1006	1014	1022	rBV	1134181	1843032	34.18%	3.009%
31	9.222	1035	1043	1046	rBV9	5996	12602	0.23%	0.021%
32	9.446	1077	1081	1087	rVB2	12527	17067	0.32%	0.028%
33	9.769	1127	1136	1149	rBV	805717	1376888	25.53%	2.248%
34	9.905	1154	1159	1166	rBV2	19350	37600	0.70%	0.061%
35	10.040	1181	1182	1188	rVB6	6689	9109	0.17%	0.015%
36	10.140	1194	1199	1203	rVB5	10706	18570	0.34%	0.030%

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Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
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37	10.305	1219	1227	1238	rBV	1324982	2188337	40.58%	3.572%
38	10.552	1265	1269	1276	rBV7	6608	12936	0.24%	0.021%
39	10.687	1284	1292	1301	rBV	1086656	1876695	34.80%	3.064%
40	10.828	1307	1316	1335	rBV	997708	1799732	33.37%	2.938%
41	11.234	1380	1385	1392	rBV10	6671	15155	0.28%	0.025%
42	11.440	1416	1420	1424	rBV5	7615	11851	0.22%	0.019%
43	11.505	1424	1431	1434	rBV8	4737	10750	0.20%	0.018%
44	12.116	1530	1535	1539	rVV2	12687	18252	0.34%	0.030%
45	12.216	1545	1552	1558	rBV	95480	168006	3.12%	0.274%
46	12.269	1558	1561	1568	rVB3	22207	39630	0.73%	0.065%
47	12.934	1669	1674	1678	rVB7	6442	12973	0.24%	0.021%
48	13.357	1736	1746	1752	rBV3	30150	48989	0.91%	0.080%
49	13.434	1752	1759	1766	rVV	48254	85035	1.58%	0.139%
50	13.493	1766	1769	1777	rVB8	6890	14882	0.28%	0.024%
51	13.951	1839	1847	1856	rBV	2161725	3068030	56.89%	5.009%
52	14.222	1883	1893	1906	rBV	2530721	3706503	68.73%	6.051%
53	14.434	1926	1929	1933	rVB5	5839	9991	0.19%	0.016%
54	14.528	1937	1945	1953	rVV	1463405	2105582	39.05%	3.437%
55	14.604	1953	1958	1959	rVV5	5501	9167	0.17%	0.015%
56	14.728	1972	1979	2000	rBV	1041433	1551912	28.78%	2.534%
57	14.893	2003	2007	2012	rVV6	18156	34389	0.64%	0.056%
58	14.957	2012	2018	2023	rVB7	26477	52783	0.98%	0.086%
59	15.522	2106	2114	2121	rBV	3077754	4417479	81.92%	7.212%
60	15.593	2123	2126	2129	rVB4	9330	9988	0.19%	0.016%
61	15.645	2129	2135	2145	rBV	822457	1125514	20.87%	1.837%
62	15.763	2151	2155	2164	rVB4	14468	26865	0.50%	0.044%
63	16.093	2207	2211	2215	rBV6	4850	7509	0.14%	0.012%
64	16.310	2244	2248	2253	rVB8	10140	15004	0.28%	0.024%
65	16.692	2305	2313	2315	rBV8	7106	12455	0.23%	0.020%
66	16.828	2331	2336	2342	rBV3	24843	36070	0.67%	0.059%
67	17.051	2370	2374	2379	rBV7	4580	9219	0.17%	0.015%
68	17.281	2406	2413	2418	rBV	1570203	2276020	42.21%	3.716%
69	17.316	2418	2419	2423	rVV	46096	51450	0.95%	0.084%
70	17.381	2423	2430	2441	rVV	2968195	4392514	81.46%	7.171%
71	17.457	2441	2443	2444	rVV2	12588	11910	0.22%	0.019%
72	17.481	2444	2447	2451	rVB3	28888	38098	0.71%	0.062%
73	17.634	2469	2473	2475	rBV4	8714	10681	0.20%	0.017%
74	17.669	2477	2479	2485	rVB7	8855	13775	0.26%	0.022%
75	17.798	2496	2501	2504	rBV6	5883	11932	0.22%	0.019%
76	17.963	2527	2529	2534	rBV6	7951	10680	0.20%	0.017%

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77	18.063	2540	2546	2551	rBV7	10208	19517	0.36%	0.032%
78	18.192	2563	2568	2578	rBV	414938	607972	11.27%	0.993%
79	18.263	2578	2580	2589	rVV2	19796	34978	0.65%	0.057%
80	18.345	2592	2594	2599	rVB5	8013	13303	0.25%	0.022%
81	18.492	2615	2619	2621	rBV5	7996	14145	0.26%	0.023%
82	18.622	2638	2641	2645	rBV5	13498	16150	0.30%	0.026%
83	18.663	2645	2648	2652	rBV5	12954	19028	0.35%	0.031%
84	18.763	2662	2665	2669	rVB2	17452	19913	0.37%	0.033%
85	18.863	2679	2682	2686	rBV6	6150	10021	0.19%	0.016%
86	18.992	2701	2704	2708	rVB4	13056	16008	0.30%	0.026%
87	19.081	2716	2719	2724	rVV6	27548	39559	0.73%	0.065%
88	19.239	2739	2746	2750	rBV6	54695	104624	1.94%	0.171%
89	19.310	2754	2758	2759	rVV	49447	64019	1.19%	0.105%
90	19.339	2760	2763	2768	rVB	117630	173838	3.22%	0.284%
91	19.475	2782	2786	2792	rBV	175892	233582	4.33%	0.381%
92	19.616	2808	2810	2814	rBV5	15791	19169	0.36%	0.031%
93	19.675	2814	2820	2830	rBV	3987787	5392517	100.00%	8.803%
94	19.933	2862	2864	2871	rVB6	18809	25021	0.46%	0.041%
95	20.210	2908	2911	2914	rVB4	21290	21366	0.40%	0.035%
96	21.204	3075	3080	3085	rBV	462977	608516	11.28%	0.993%
97	21.475	3120	3126	3131	rBV	1694753	2284363	42.36%	3.729%
98	23.698	3497	3504	3517	rVB2	2619312	5077328	94.16%	8.289%
99	23.851	3523	3530	3541	rVB	1121102	2378396	44.11%	3.883%
100	24.616	3654	3660	3670	rBV3	153221	368182	6.83%	0.601%

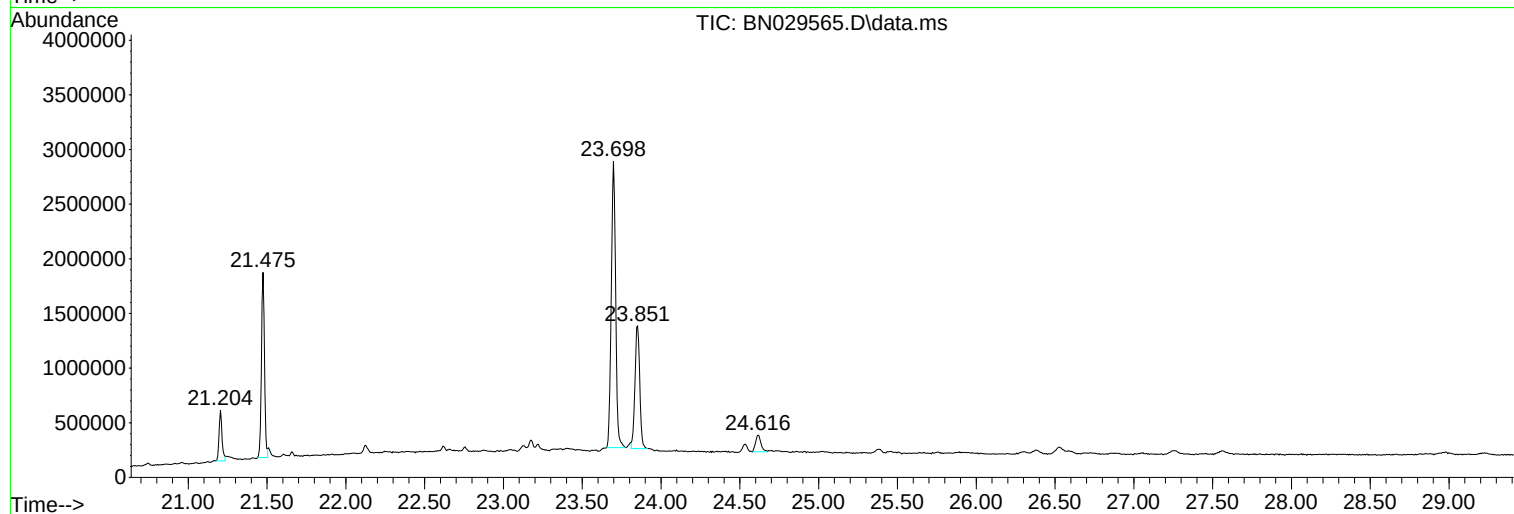
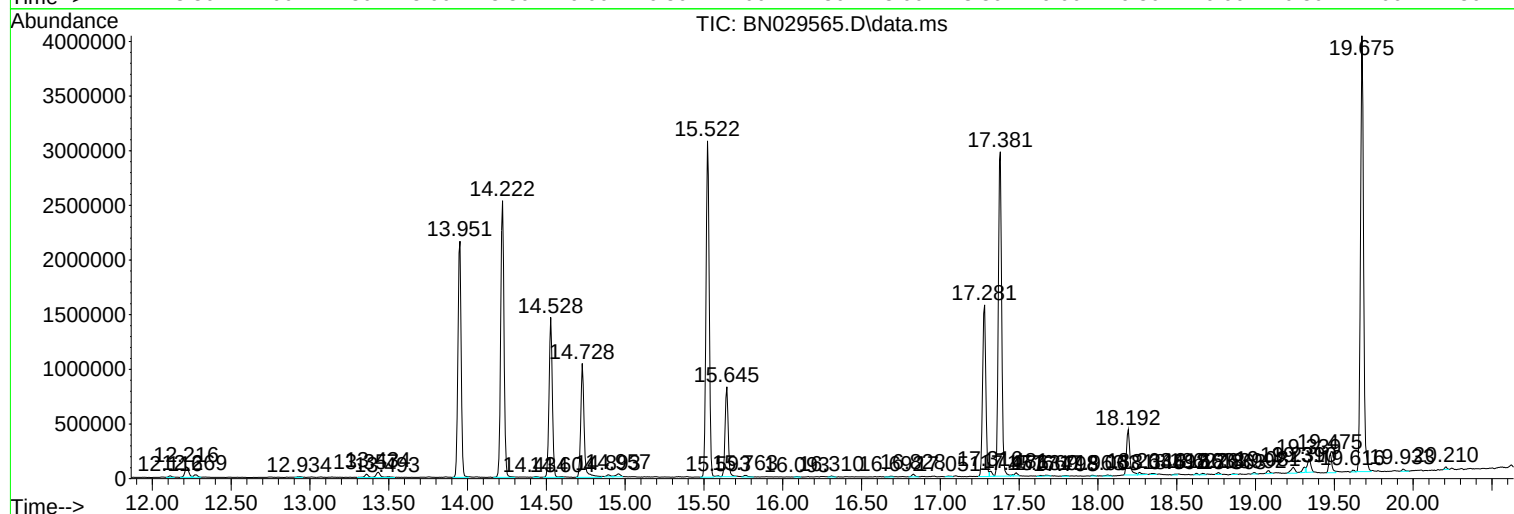
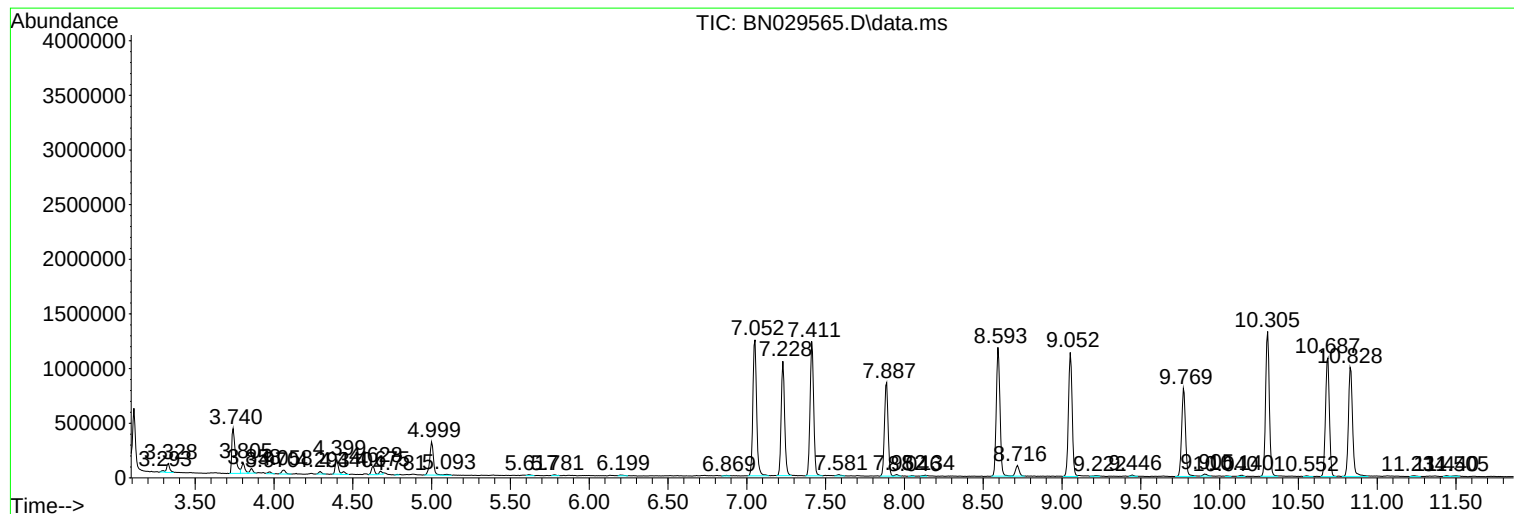
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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



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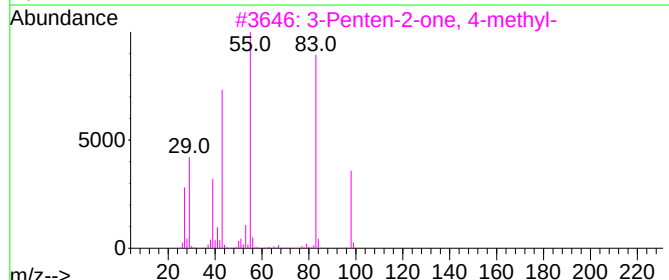
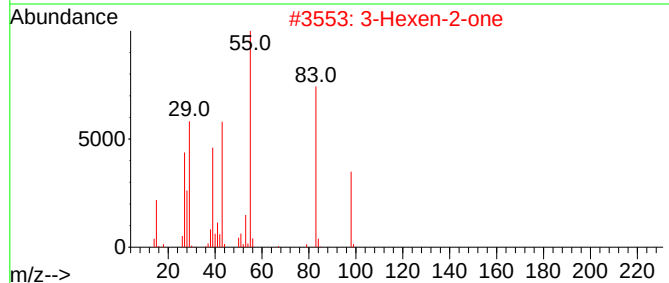
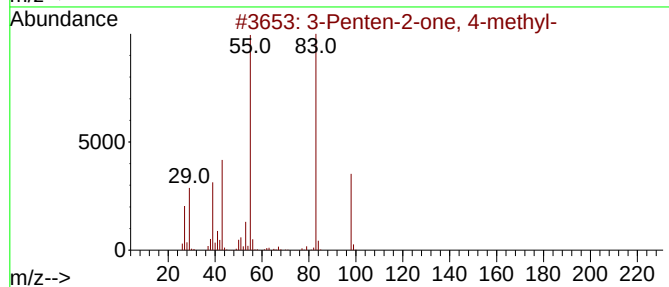
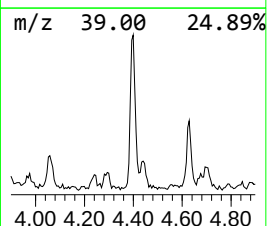
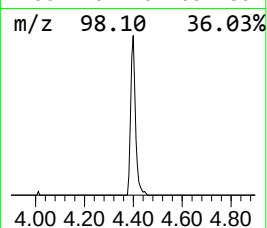
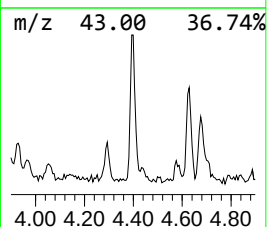
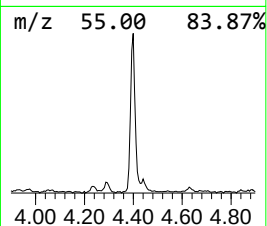
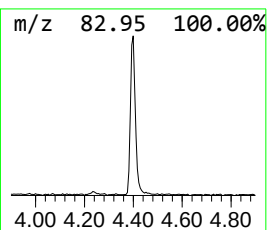
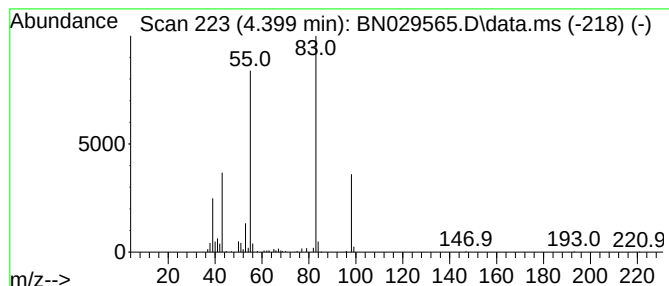
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.399	2.54 ng/ul	174724	1,4-Dichlorobenzene-d4	7.887

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
4		3-Hexen-2-one	98	C6H10O	000763-93-9	90
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90



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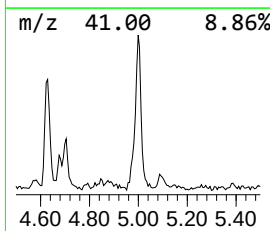
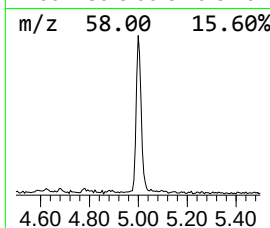
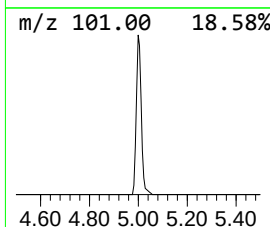
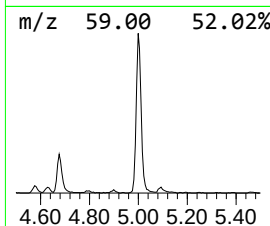
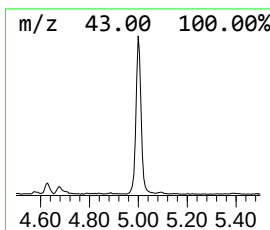
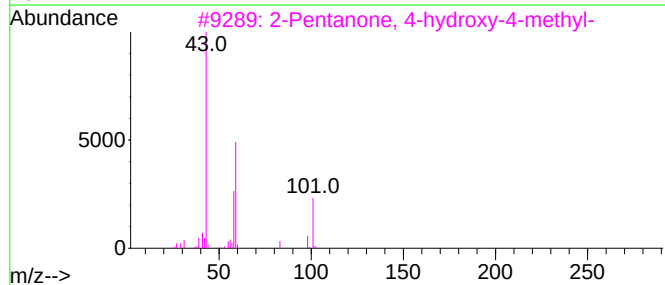
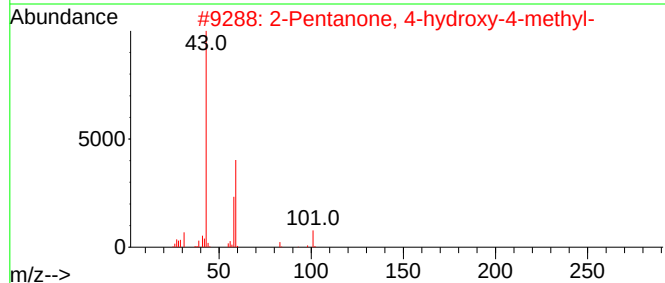
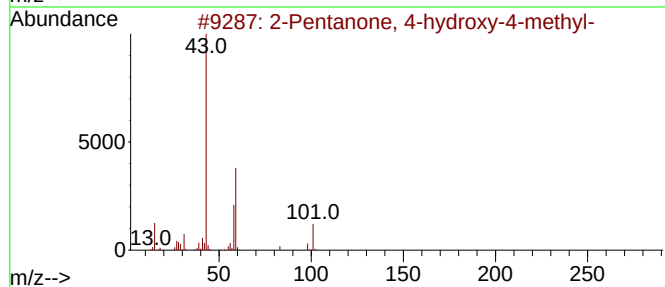
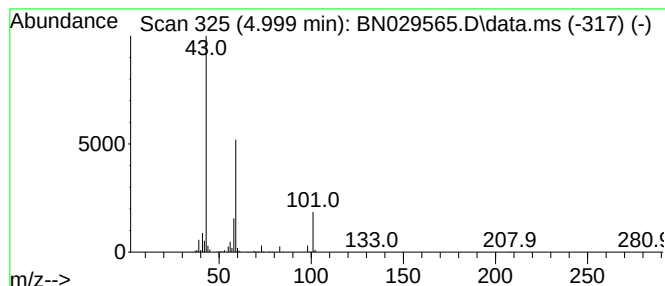
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.999	7.17 ng/ul	492675	1,4-Dichlorobenzene-d4	7.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		



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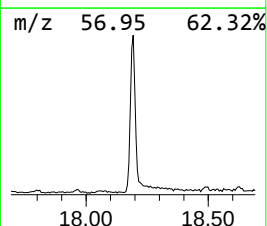
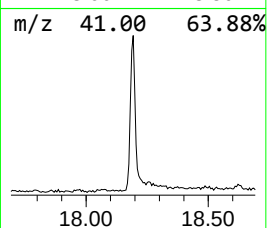
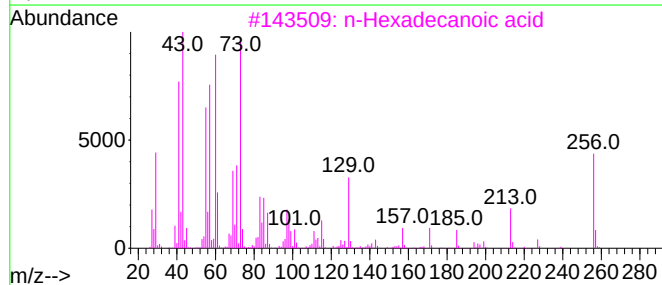
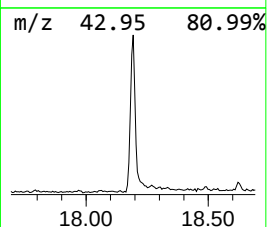
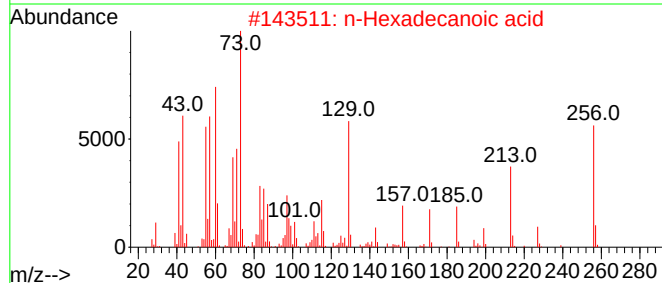
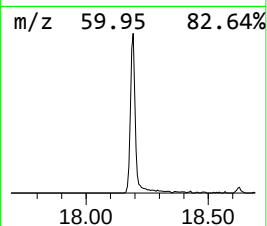
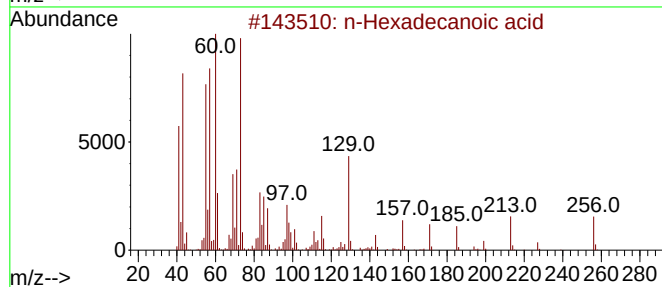
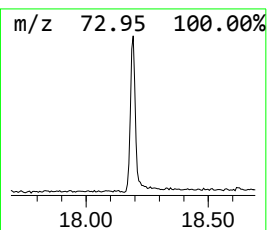
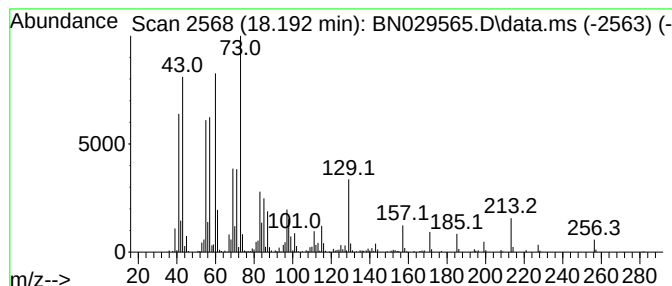
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.192	5.34 ng/ul	607972	Phenanthrene-d10		17.281	
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	99
4	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
5	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029565.D
Acq On : 08 Feb 2024 03:06
Operator : MA/JU
Sample : P1303-20
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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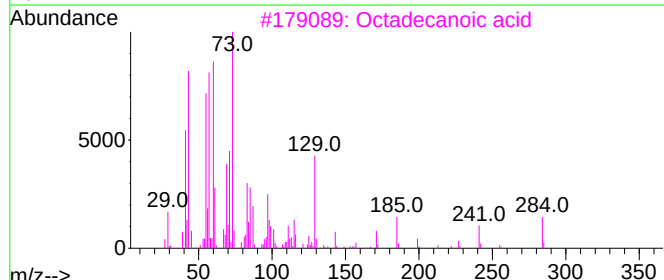
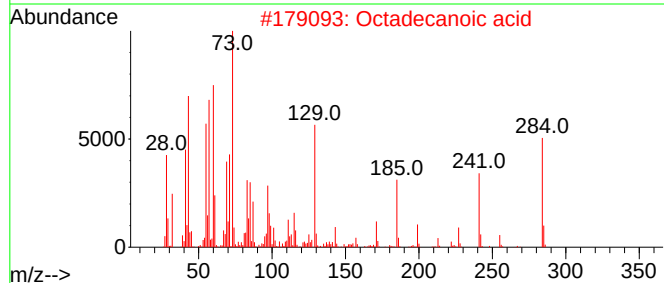
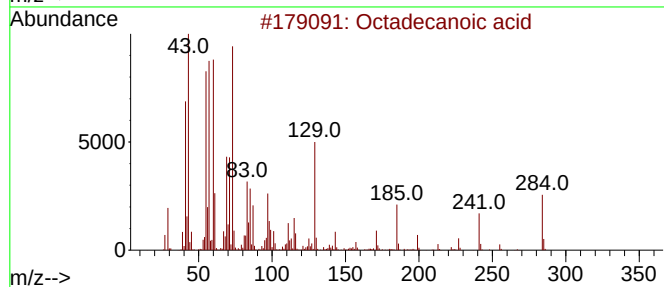
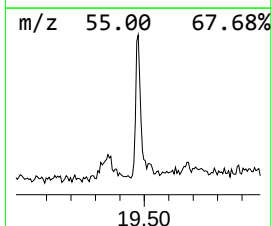
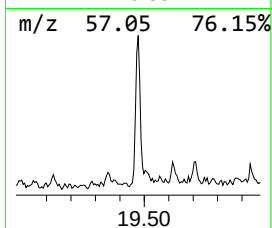
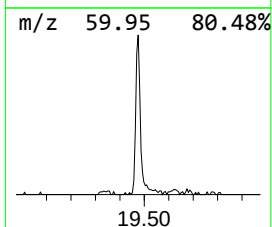
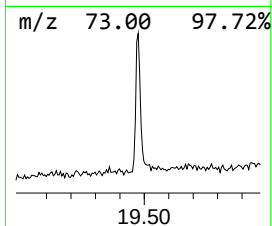
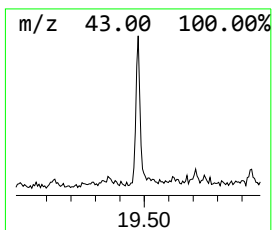
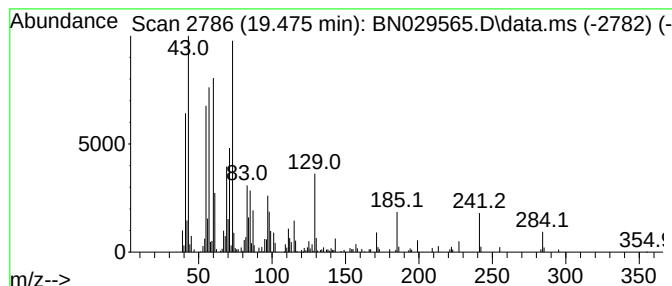
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.475	2.05 ng/ul	233582	Chrysene-d12	21.475

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	97
4			Octadecanoic acid	284	C18H36O2	000057-11-4	97
5			Octadecanoic acid	284	C18H36O2	000057-11-4	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029565.D
Acq On : 08 Feb 2024 03:06
Operator : MA/JU
Sample : P1303-20
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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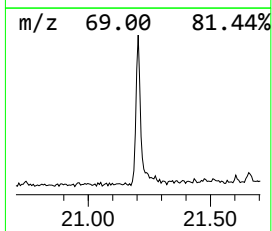
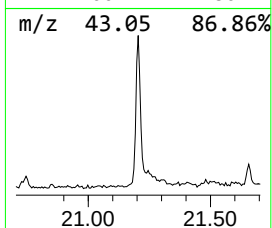
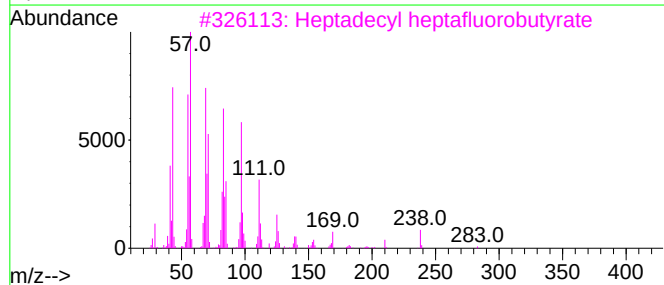
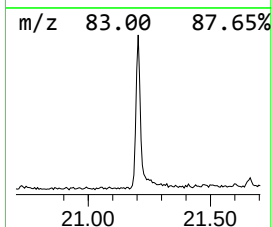
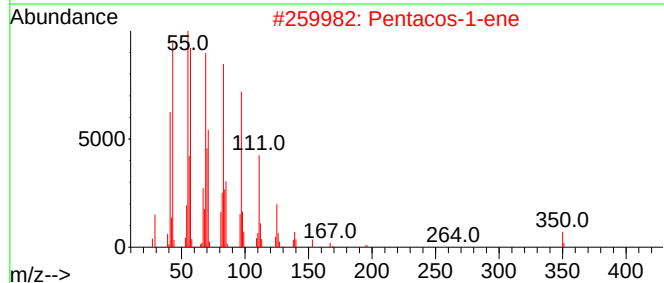
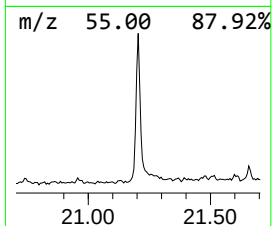
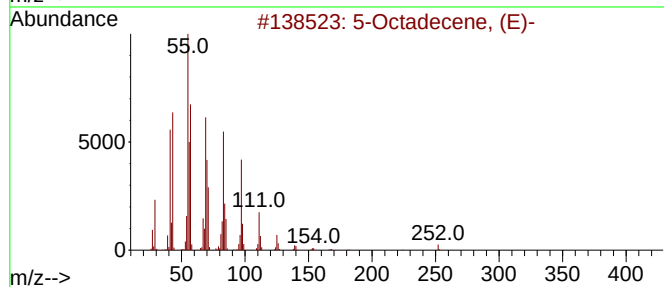
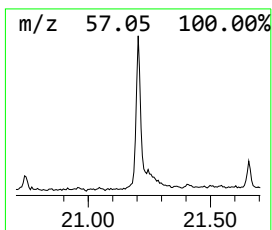
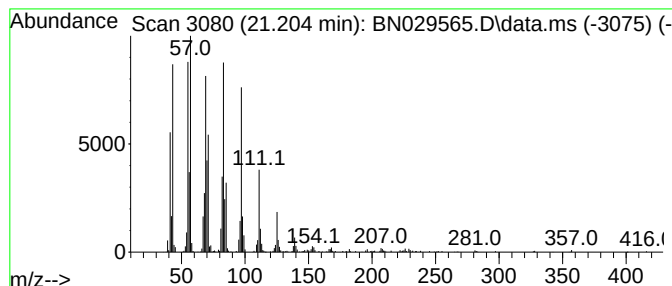
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	5.33 ng/ul	608516	Chrysene-d12	21.475

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Octadecene, (E)-	252	C18H36	007206-21-5	94
2			Pentacos-1-ene	350	C25H50	016980-85-1	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5			1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029565.D
Acq On : 08 Feb 2024 03:06
Operator : MA/JU
Sample : P1303-20
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0FJ7

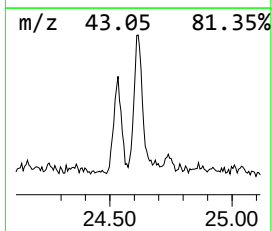
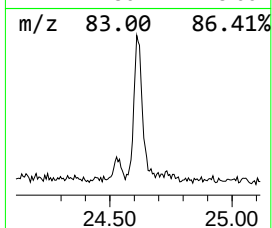
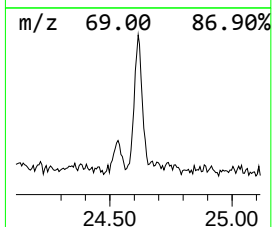
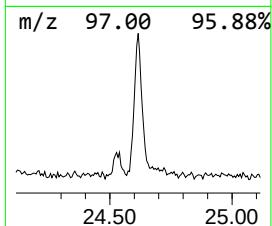
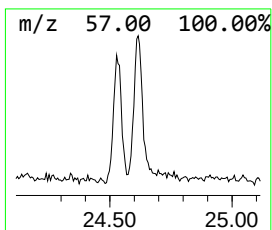
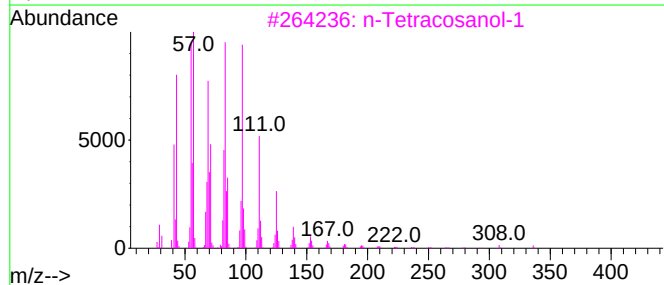
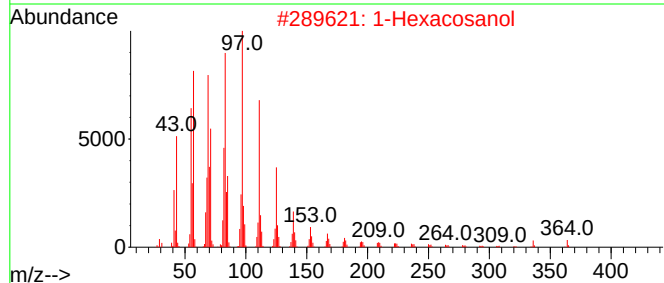
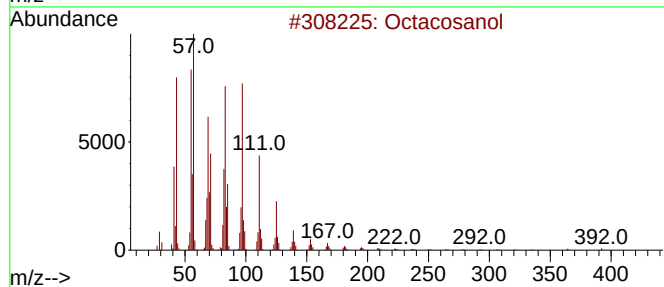
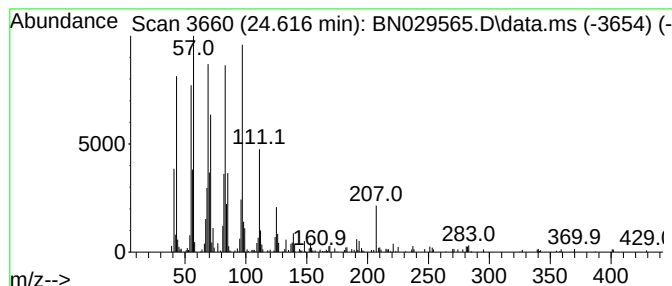
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.616	3.10 ng/ul	368182	Perylene-d12	23.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosanol	410	C28H58O	000557-61-9	93
2			1-Hexacosanol	382	C26H54O	000506-52-5	91
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4			Triacontan-15-ol	438	C30H62O	031849-26-0	90
5			1-Hexacosene	364	C26H52	018835-33-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN020724\
Data File : BN029565.D
Acq On : 08 Feb 2024 03:06
Operator : MA/JU
Sample : P1303-20
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
C0FJ7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN020724.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
3-Penten-2-one,...	4.399	2.5	ng/ul	174724	1	7.887	1374490	20.0
2-Pentanone, 4-...	4.999	7.2	ng/ul	492675	1	7.887	1374490	20.0
n-Hexadecanoic ...	18.192	5.3	ng/ul	607972	4	17.281	2276020	20.0
Octadecanoic acid	19.475	2.0	ng/ul	233582	5	21.475	2284360	20.0
(DEL) Alkane: S...	21.204	5.3	ng/ul	608516	5	21.475	2284360	20.0
Octacosanol	24.616	3.1	ng/ul	368182	6	23.851	2378400	20.0