

Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN012221\
 Data File : BN013459.D
 Acq On : 22 Jan 2021 15:23
 Operator : CG/JU
 Sample : M1050-07
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 X2X39

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0.1 % of largest Peak
 Max Peaks: 100
 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-BN012221.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.181	13	16	23	rVB	85715	114435	0.47%	0.040%
2	3.499	66	70	78	rBV	64674	95229	0.39%	0.033%
3	3.563	78	81	88	rVV	1185196	1694692	6.98%	0.593%
4	3.616	88	90	102	rVB	117359	164915	0.68%	0.058%
5	3.887	131	136	140	rVB	57407	78166	0.32%	0.027%
6	4.187	182	187	203	rBV	7198047	9551632	39.34%	3.342%
7	4.763	280	285	294	rBV	762310	1021194	4.21%	0.357%
8	5.363	383	387	391	rVB2	24973	37762	0.16%	0.013%
9	5.810	459	463	471	rVB	32441	49046	0.20%	0.017%
10	6.787	625	629	636	rVB	3286760	5155548	21.24%	1.804%
11	6.928	646	653	664	rBV	1170060	1831651	7.54%	0.641%
12	7.116	678	685	694	rBV	1681277	2500197	10.30%	0.875%
13	7.581	757	764	772	rBV	1807499	2771350	11.42%	0.970%
14	8.281	870	883	894	rBV	1730154	2733034	11.26%	0.956%
15	8.722	950	958	961	rBV	1282398	2154316	8.87%	0.754%
16	8.763	961	965	976	rVB	2382344	3681523	15.16%	1.288%
17	9.175	1030	1035	1040	rBV	52382	76603	0.32%	0.027%
18	9.281	1046	1053	1063	rBV	3662920	5866526	24.16%	2.052%
19	9.434	1072	1079	1089	rBV	1074959	1691772	6.97%	0.592%
20	9.593	1101	1106	1117	rVB	94257	140806	0.58%	0.049%
21	9.969	1162	1170	1182	rBV	1747314	2809186	11.57%	0.983%
22	10.345	1226	1234	1238	rBV	2330603	3944700	16.25%	1.380%
23	10.392	1238	1242	1250	rVV	6198289	10194415	41.99%	3.566%
24	10.481	1250	1257	1267	rVV	1380227	2291129	9.44%	0.802%
25	11.881	1489	1495	1502	rVV2	88334	174329	0.72%	0.061%
26	11.939	1502	1505	1510	rVB	30156	41471	0.17%	0.015%
27	12.016	1510	1518	1527	rBV	5542889	8801347	36.25%	3.079%
28	12.234	1545	1555	1562	rVB2	94960	171178	0.71%	0.060%
29	12.634	1616	1623	1641	rVB	4695570	6934209	28.56%	2.426%
30	13.045	1686	1693	1701	rVB	5445625	7803474	32.14%	2.730%
31	13.128	1701	1707	1714	rBV	78779	121006	0.50%	0.042%
32	13.633	1786	1793	1798	rBV	3231861	4354429	17.94%	1.523%
33	13.681	1798	1801	1808	rVB	442048	561678	2.31%	0.196%
34	13.904	1832	1839	1842	rBV	3321830	5450451	22.45%	1.907%

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35	13.933	1842	1844	1854	rVB	3336772	4113795	16.95%	1.439%
36	14.145	1875	1880	1885	rBV	18941	27442	0.11%	0.010%
37	14.216	1885	1892	1899	rVV	3074321	4364525	17.98%	1.527%
38	14.281	1899	1903	1910	rVB2	26413	40175	0.17%	0.014%
39	14.416	1917	1926	1940	rBV	1585210	2174193	8.96%	0.761%
40	14.622	1951	1961	1970	rVB	6396109	9417550	38.79%	3.295%
41	14.845	1995	1999	2005	rBV6	47750	73277	0.30%	0.026%
42	15.057	2029	2035	2041	rBV	5346439	7200419	29.66%	2.519%
43	15.104	2041	2043	2048	rVB2	51508	53065	0.22%	0.019%
44	15.216	2055	2062	2068	rBV	4681562	6478032	26.68%	2.266%
45	15.333	2076	2082	2091	rBV	1153923	1572240	6.48%	0.550%
46	15.457	2098	2103	2107	rBV	51234	68606	0.28%	0.024%
47	16.004	2192	2196	2201	rVB6	19411	32803	0.14%	0.011%
48	16.133	2213	2218	2223	rBV6	16529	28668	0.12%	0.010%
49	16.275	2236	2242	2250	rVV	4163403	5875811	24.20%	2.056%
50	16.616	2295	2300	2313	rBV	4977125	6752412	27.81%	2.362%
51	16.757	2320	2324	2329	rVB3	36744	46635	0.19%	0.016%
52	16.969	2353	2360	2365	rBV	3028241	4338976	17.87%	1.518%
53	17.010	2365	2367	2371	rVV	108355	113075	0.47%	0.040%
54	17.069	2371	2377	2379	rVV2	4894353	7171242	29.54%	2.509%
55	17.104	2379	2383	2393	rVB	8695101	12053893	49.65%	4.217%
56	17.374	2422	2429	2435	rBV	8990482	12658848	52.14%	4.429%
57	17.592	2460	2466	2472	rBV4	54091	80193	0.33%	0.028%
58	17.886	2512	2516	2520	rBV2	105499	156387	0.64%	0.055%
59	17.921	2520	2522	2525	rVV2	40239	48477	0.20%	0.017%
60	17.957	2525	2528	2531	rVB	27814	34776	0.14%	0.012%
61	18.192	2564	2568	2572	rVV	57311	77558	0.32%	0.027%
62	18.386	2592	2601	2609	rBV3	79404	148564	0.61%	0.052%
63	18.757	2662	2664	2669	rVB5	17504	24571	0.10%	0.009%
64	18.833	2672	2677	2681	rVB6	31010	50333	0.21%	0.018%
65	19.039	2700	2712	2719	rBV	8388119	11810847	48.65%	4.132%
66	19.180	2732	2736	2740	rBV5	40666	55718	0.23%	0.019%
67	19.257	2745	2749	2753	rVB	47483	63203	0.26%	0.022%
68	19.368	2762	2768	2775	rBV2	5713871	7792596	32.10%	2.726%
69	20.321	2927	2930	2934	rBV4	27513	33109	0.14%	0.012%
70	20.910	3025	3030	3042	rBV2	877197	1218923	5.02%	0.426%
71	21.115	3060	3065	3068	rBV	8919547	9546560	39.32%	3.340%

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72	21.157	3068	3072	3085	rVB2	8250385	13520364	55.69%	4.730%
73	21.786	3175	3179	3183	rBV2	117831	185233	0.76%	0.065%
74	21.980	3207	3212	3219	rBV	8928251	10589744	43.62%	3.705%
75	22.233	3252	3255	3259	rVB2	121182	156377	0.64%	0.055%
76	22.733	3336	3340	3345	rBV	243135	343135	1.41%	0.120%
77	23.215	3415	3422	3430	rBV	4196709	7451813	30.69%	2.607%
78	23.286	3430	3434	3439	rVV	275648	455384	1.88%	0.159%
79	23.357	3439	3446	3464	rVB	2273515	4282973	17.64%	1.498%
80	23.915	3536	3541	3548	rVB	301397	544826	2.24%	0.191%
81	24.639	3659	3664	3671	rBV2	211725	397779	1.64%	0.139%
82	25.551	3804	3819	3839	rVB3	7906957	24277227	100.00%	8.493%
83	26.209	3919	3931	3943	rVB2	4336767	12782592	52.65%	4.472%

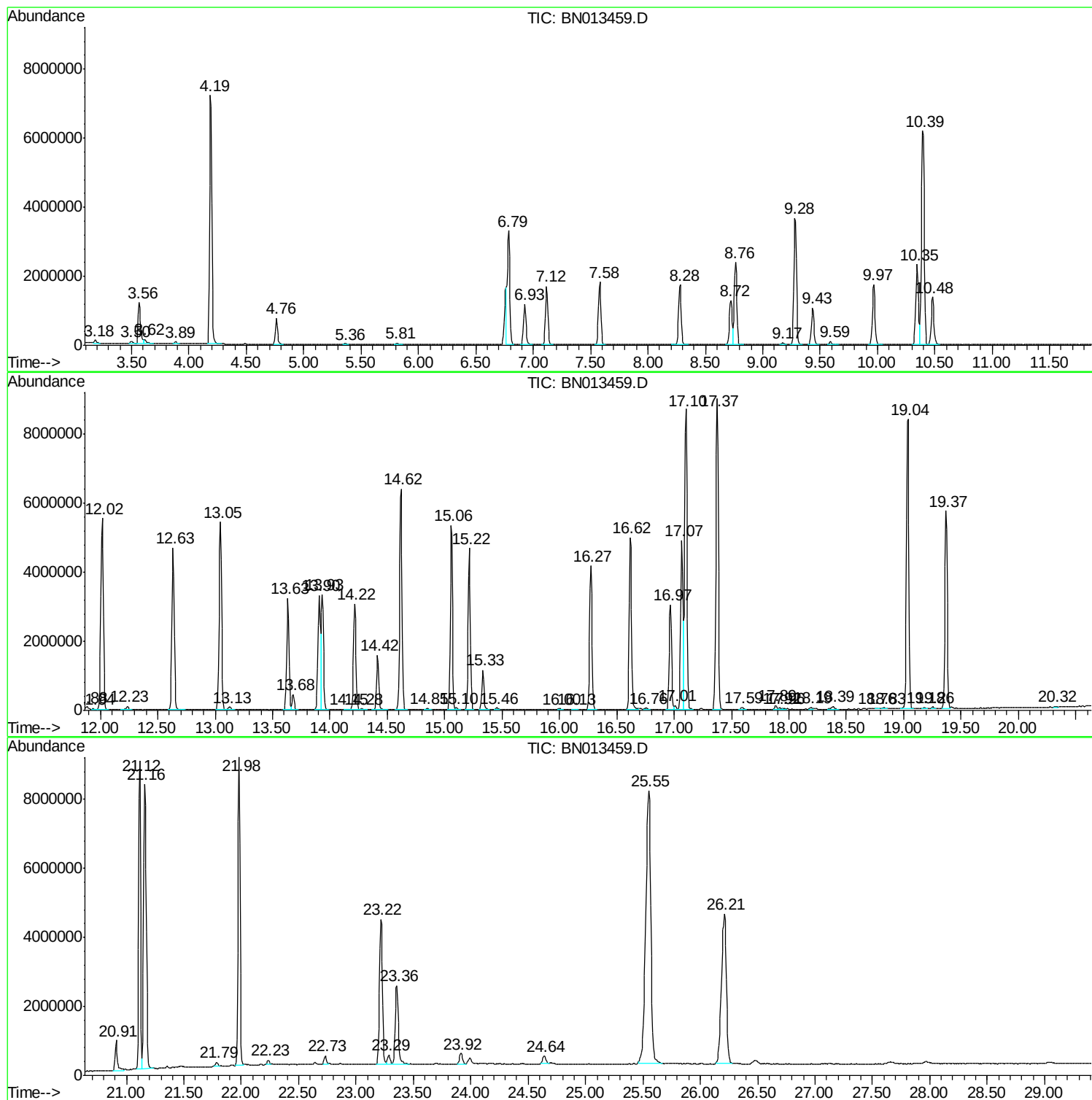
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SFAM-EPA-BN012221.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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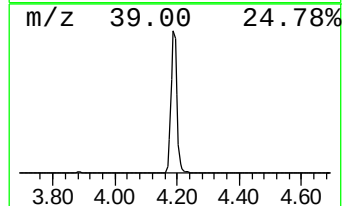
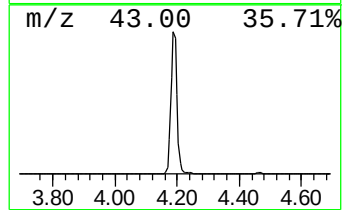
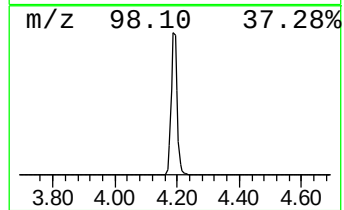
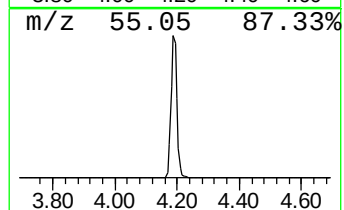
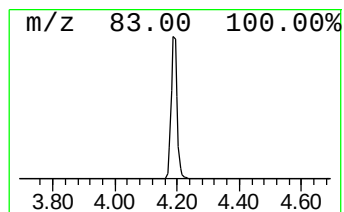
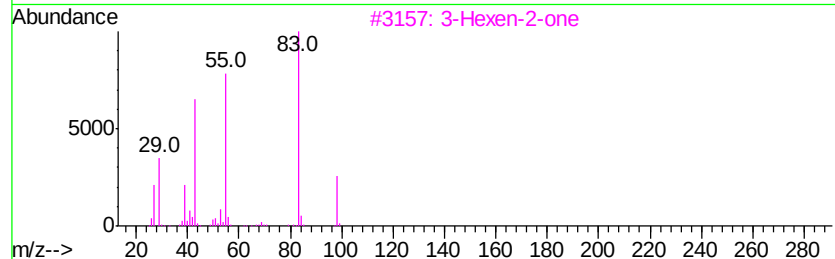
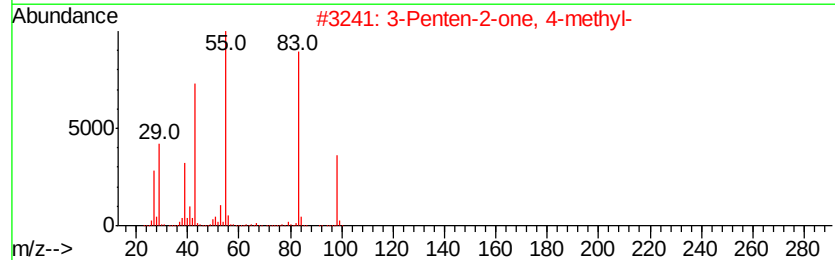
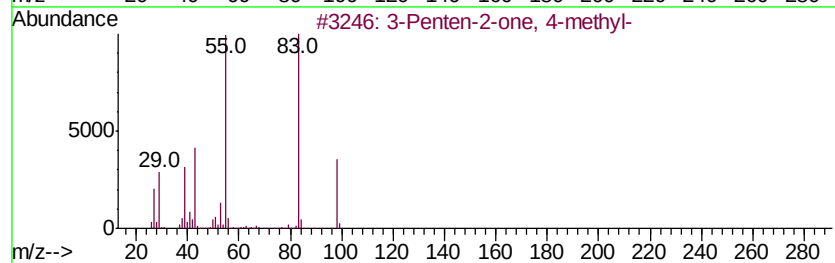
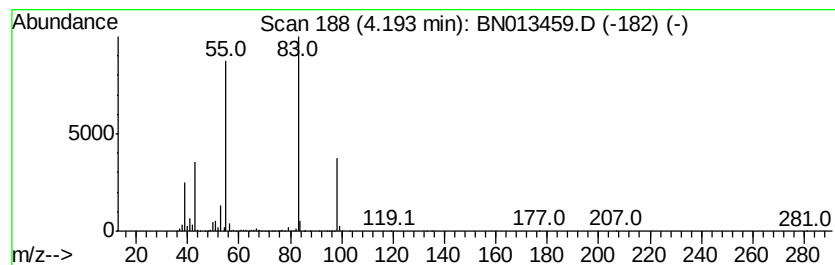
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SFAM-EPA-BN012221.M
 Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.19	68.93 ng/ul	9551630	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		3-Hexen-2-one	98	C6H10O	000763-93-9	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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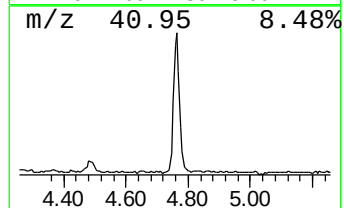
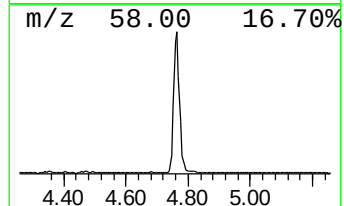
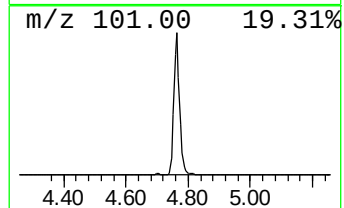
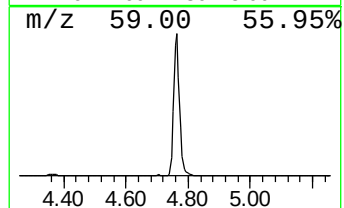
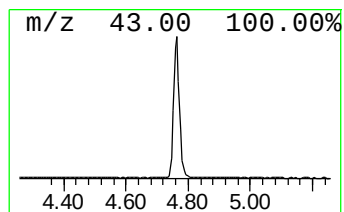
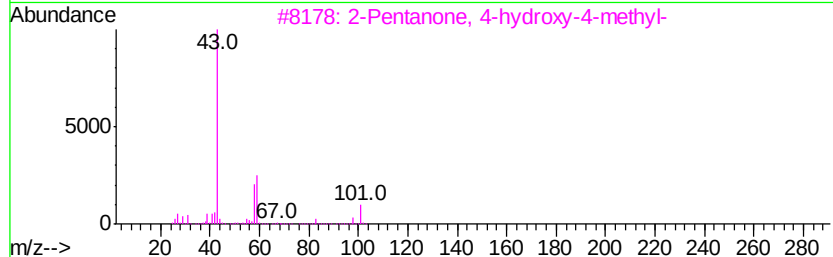
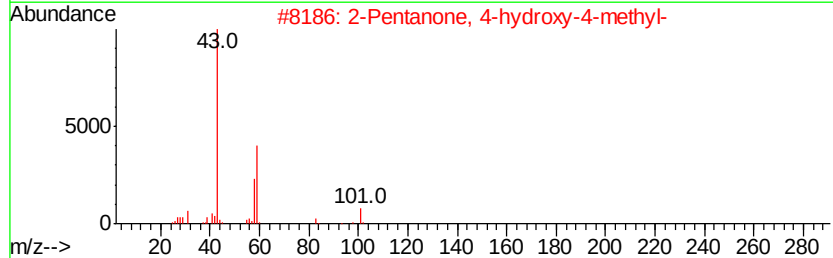
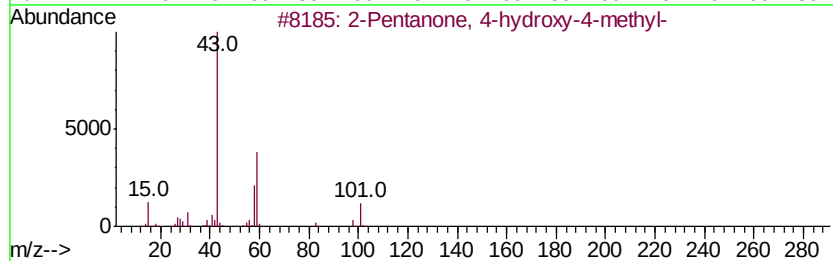
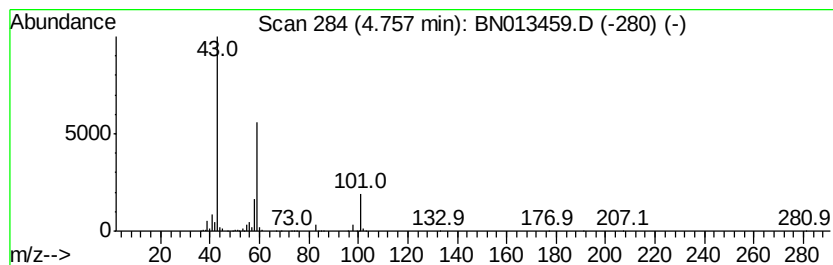
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	7.37 ng/ul	1021190	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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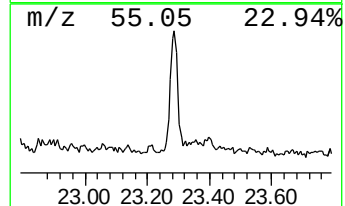
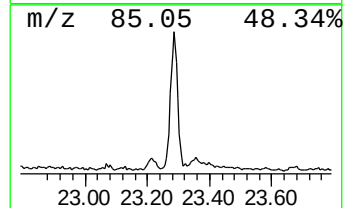
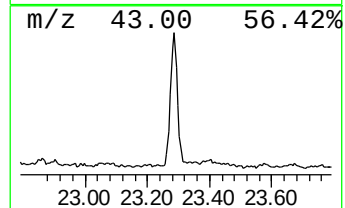
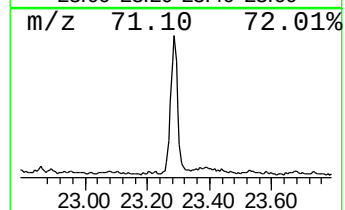
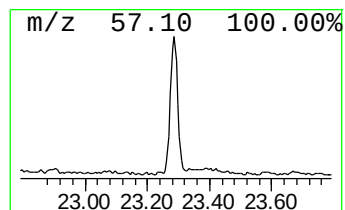
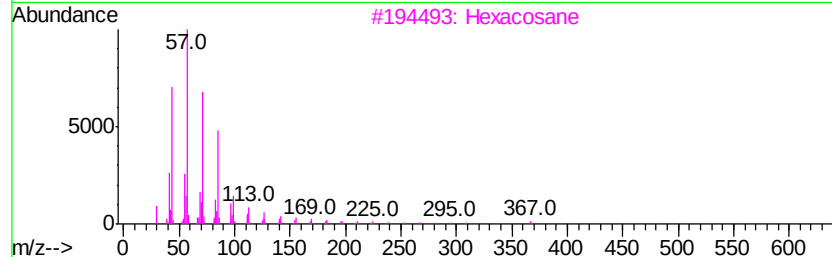
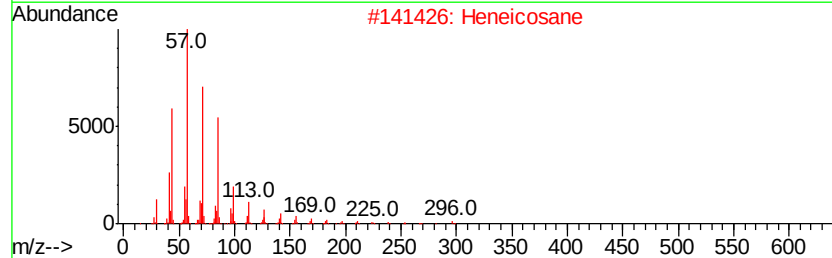
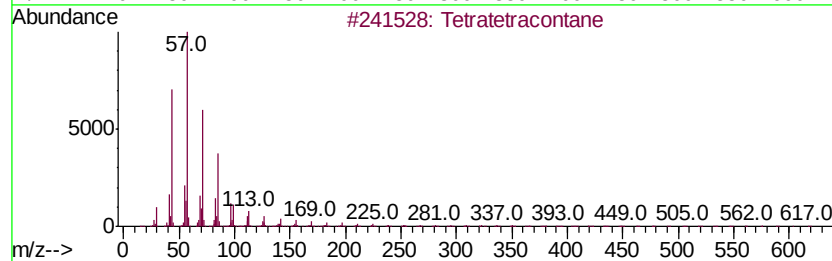
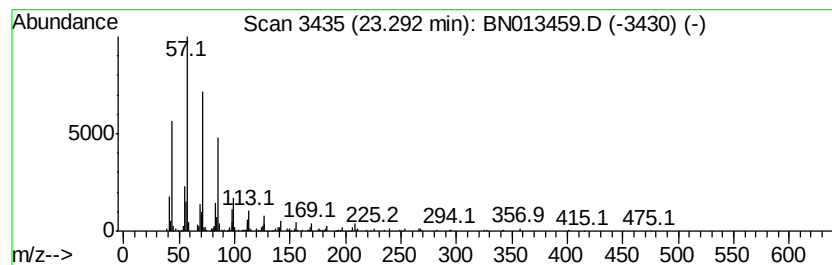
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	2.13 ng/ul	455384	Perylene-d12	23.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	90
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heptadecane	240	C17H36	000629-78-7	87
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87



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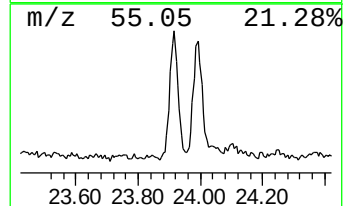
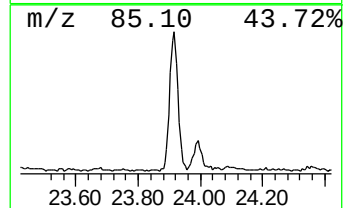
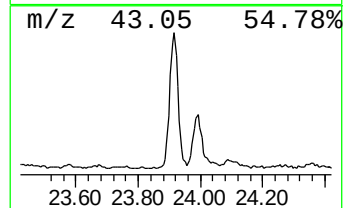
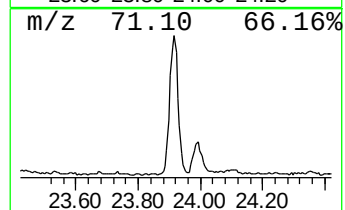
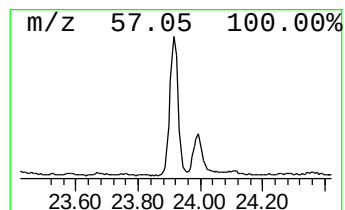
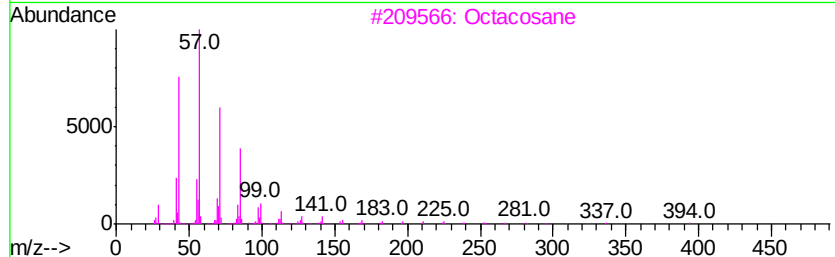
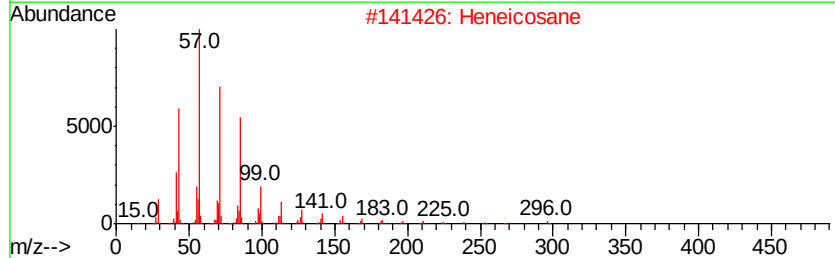
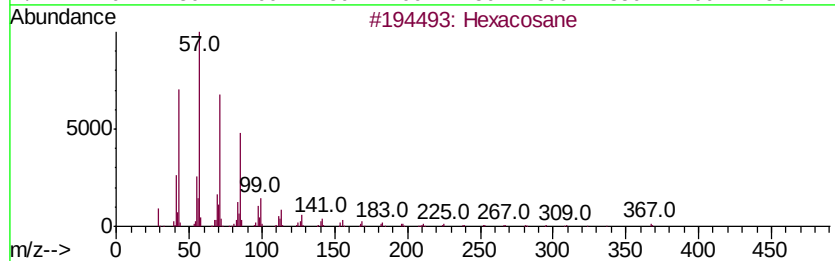
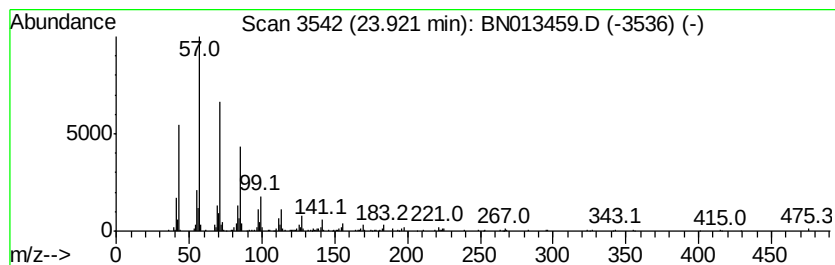
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
23.92	2.54 ng/ul	544826	Perylene-d12	23.36

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA N\DATA\BN012221\
Data File : BN013459.D
Acq On : 22 Jan 2021 15:23
Operator : CG/JU
Sample : M1050-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
X2X39

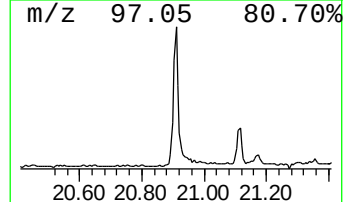
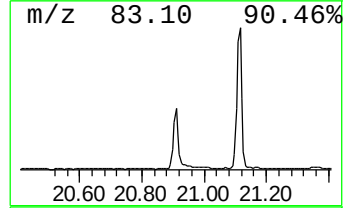
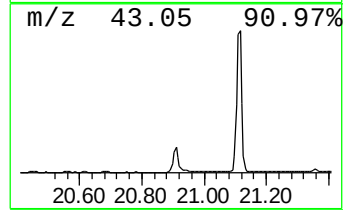
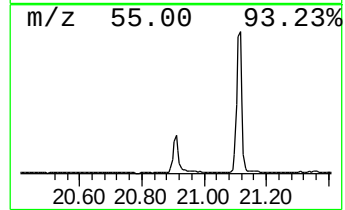
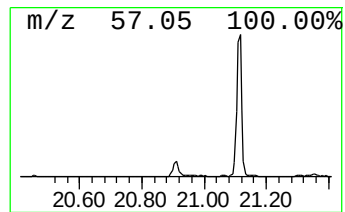
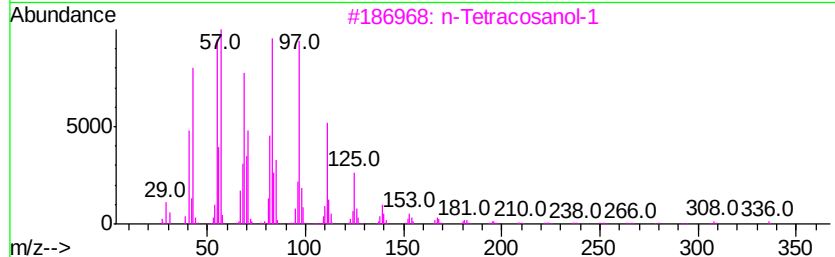
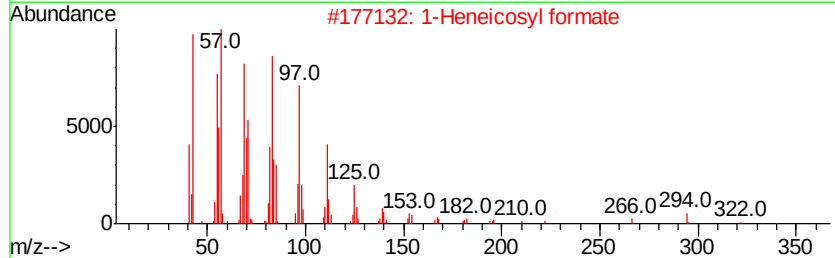
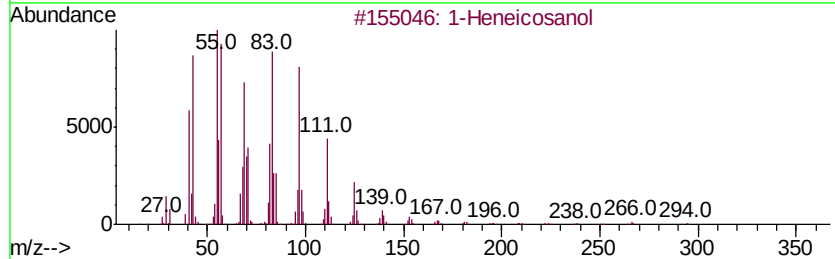
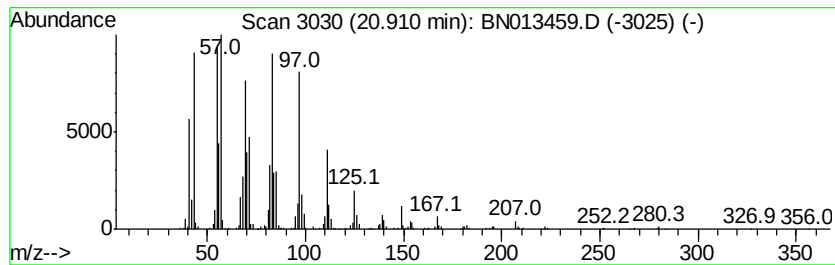
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	1.80 ng/ul	1218920	Chrysene-d12	21.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	93
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		1-Eicosene	280	C20H40	003452-07-1	91
5		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_N\DATA\BN012221\
Data File : BN013459.D
Acq On : 22 Jan 2021 15:23
Operator : CG/JU
Sample : M1050-07
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
X2X39

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\SFAM-EPA-BN012221.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.19	68.9	ng/ul	9551630	1	7.58	2771350	20.0
2-Pentanone, 4-hy...	4.76	7.4	ng/ul	1021190	1	7.58	2771350	20.0
(DEL) Alkane: Str...	23.29	2.1	ng/ul	455384	6	23.36	4282970	20.0
(DEL) Alkane: Str...	23.92	2.5	ng/ul	544826	6	23.36	4282970	20.0
1-Heneicosanol	20.91	1.8	ng/ul	1218920	5	21.17	13520400	20.0