

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
 Data File : BN022771.D
 Acq On : 19 Nov 2022 00:27
 Operator : CG/JU
 Sample : N5689-16
 Misc :
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 BGCD9

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: BN022771.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.176	29	32	37	rBV	6501	8524	0.17%	0.025%
2	3.623	106	108	124	rBV	55399	106079	2.16%	0.316%
3	3.846	142	146	154	rVB	7349	13175	0.27%	0.039%
4	3.946	159	163	166	rBV2	3444	4950	0.10%	0.015%
5	7.022	680	686	697	rVB	61673	102830	2.09%	0.307%
6	7.187	707	714	722	rBV	230634	378273	7.70%	1.128%
7	7.375	739	746	757	rBV	213592	352065	7.16%	1.050%
8	7.852	820	827	838	rVB	225085	358427	7.29%	1.069%
9	8.575	942	950	963	rBV	192086	315213	6.41%	0.940%
10	9.028	1020	1027	1039	rBV	312525	507492	10.32%	1.513%
11	9.346	1042	1081	1084	rBV	807362	4915576	100.00%	14.658%
12	9.752	1142	1150	1162	rBV	253696	422373	8.59%	1.260%
13	10.087	1179	1207	1219	rBV	374013	1784600	36.31%	5.322%
14	10.293	1236	1242	1256	rVB	344914	589038	11.98%	1.757%
15	10.669	1299	1306	1314	rBV	362124	592188	12.05%	1.766%
16	10.822	1323	1332	1341	rBV	337130	616431	12.54%	1.838%
17	10.952	1348	1354	1358	rBV2	13394	24477	0.50%	0.073%
18	10.993	1358	1361	1366	rVB4	3739	6132	0.12%	0.018%
19	11.105	1372	1380	1387	rVB4	19305	42602	0.87%	0.127%
20	11.193	1389	1395	1399	rBV3	2809	5164	0.11%	0.015%
21	11.257	1399	1406	1413	rVV3	10174	26137	0.53%	0.078%
22	11.493	1441	1446	1448	rBV	19054	30301	0.62%	0.090%
23	11.522	1448	1451	1459	rVB	24363	39253	0.80%	0.117%
24	11.687	1459	1479	1491	rBV	352610	1274732	25.93%	3.801%
25	12.269	1572	1578	1583	rVB3	5676	9721	0.20%	0.029%
26	12.422	1598	1604	1612	rBV2	10033	21130	0.43%	0.063%
27	12.969	1692	1697	1706	rVB2	3098	5181	0.11%	0.015%
28	13.693	1812	1820	1827	rBV6	2650	7569	0.15%	0.023%
29	13.940	1855	1862	1871	rVB	851556	1187736	24.16%	3.542%
30	14.216	1900	1909	1922	rBV	903314	1298783	26.42%	3.873%
31	14.404	1922	1941	1955	rBV	1243876	4005362	81.48%	11.944%
32	14.522	1955	1961	1972	rVV	617908	916892	18.65%	2.734%
33	14.746	1994	1999	2008	rBV	90679	155596	3.17%	0.464%
34	14.828	2008	2013	2022	rVB	47886	78790	1.60%	0.235%
35	14.940	2025	2032	2033	rBV3	4565	7954	0.16%	0.024%
36	15.257	2080	2086	2100	rBV2	21905	62836	1.28%	0.187%

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37	15.363	2100	2104	2108	rVB6	4240	6751	0.14%	0.020%
38	15.516	2123	2130	2139	rVB	1249694	1745134	35.50%	5.204%
39	15.645	2146	2152	2167	rBV	467308	652235	13.27%	1.945%
40	15.757	2167	2171	2177	rVB3	4689	7227	0.15%	0.022%
41	16.222	2247	2250	2255	rBV4	4778	7219	0.15%	0.022%
42	17.022	2383	2386	2389	rVV3	5160	6421	0.13%	0.019%
43	17.275	2423	2429	2435	rBV	773471	1064022	21.65%	3.173%
44	17.375	2439	2446	2461	rVV	1469257	2053822	41.78%	6.125%
45	17.739	2504	2508	2510	rBV	13451	17536	0.36%	0.052%
46	17.763	2510	2512	2522	rVB5	8183	13881	0.28%	0.041%
47	17.945	2539	2543	2548	rVB2	5969	8088	0.16%	0.024%
48	18.169	2576	2581	2587	rBV	53970	74309	1.51%	0.222%
49	18.416	2619	2623	2627	rBV6	7149	11679	0.24%	0.035%
50	18.457	2627	2630	2636	rVB3	6649	10447	0.21%	0.031%
51	19.092	2735	2738	2741	rBV4	14510	16409	0.33%	0.049%
52	19.128	2741	2744	2746	rVB4	4139	5105	0.10%	0.015%
53	19.239	2759	2763	2771	rBV3	16902	25220	0.51%	0.075%
54	19.310	2771	2775	2782	rBV2	20156	35042	0.71%	0.104%
55	19.451	2795	2799	2807	rBV	44220	67786	1.38%	0.202%
56	19.681	2832	2838	2844	rBV	1812765	2368679	48.19%	7.064%
57	21.480	3139	3144	3151	rBV	928773	1206857	24.55%	3.599%
58	23.722	3517	3525	3541	rVB2	1262848	2633391	53.57%	7.853%
59	23.874	3544	3551	3560	rVB2	600906	1223208	24.88%	3.648%

Sum of corrected areas: 33534050

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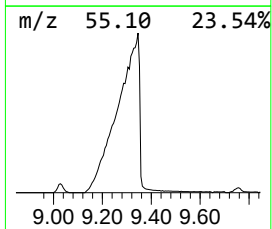
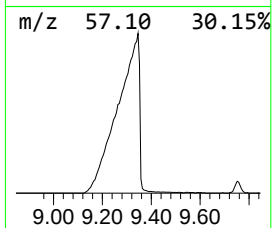
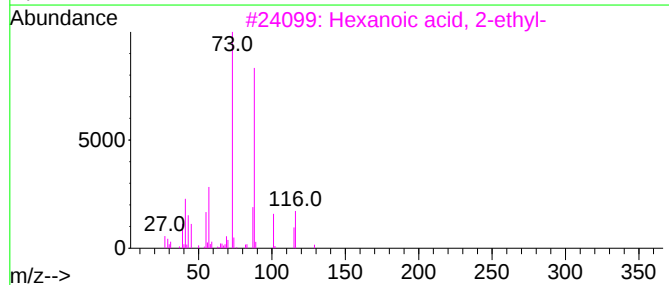
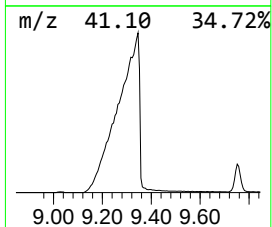
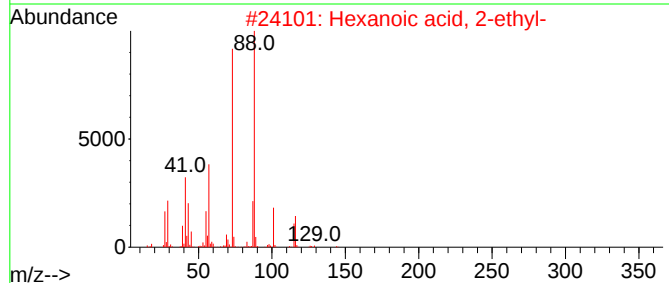
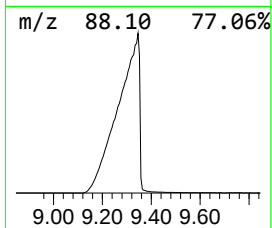
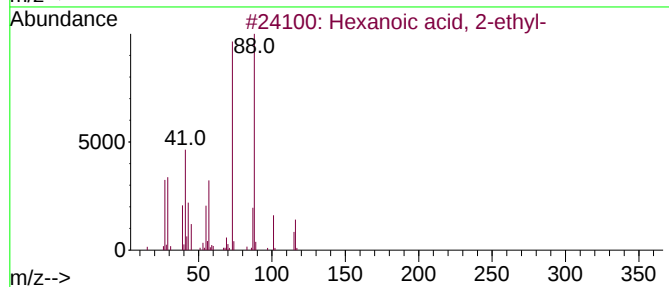
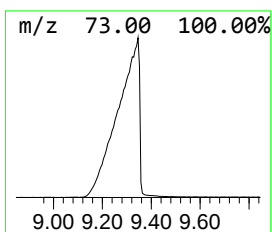
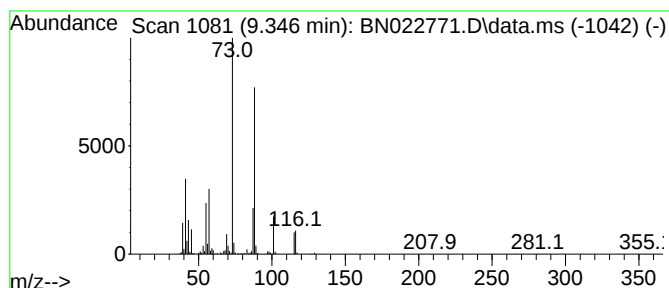
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.346	166.01 ng/ul	4915580	Naphthalene-d8	10.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
3			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
4			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	80
5			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78



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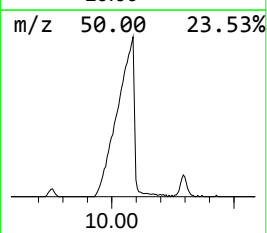
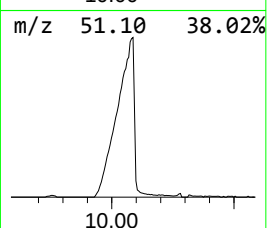
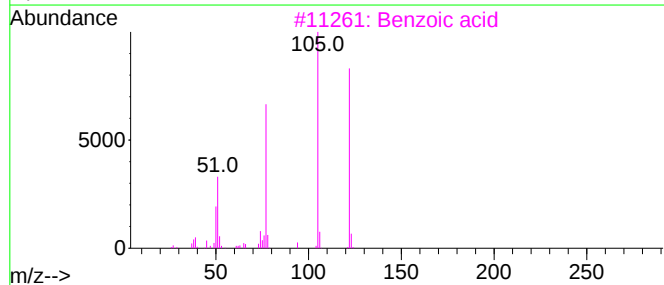
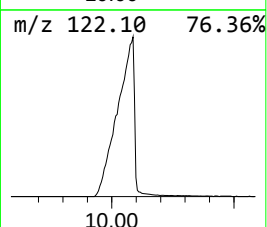
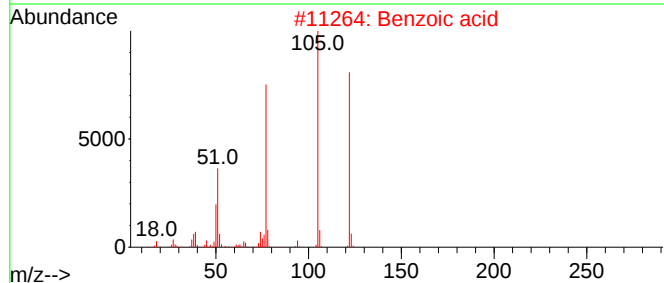
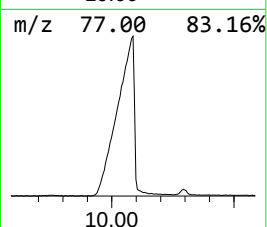
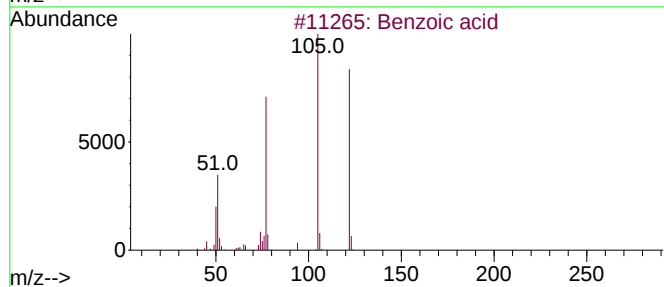
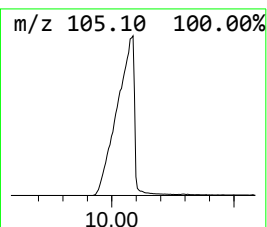
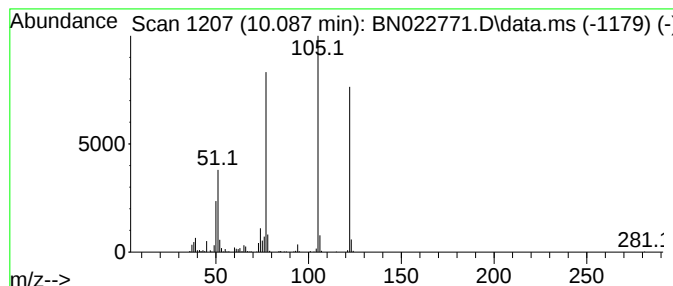
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Benzoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.087	60.27 ng/ul	1784600	Naphthalene-d8	10.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	96
2			Benzoic acid	122	C7H6O2	000065-85-0	94
3			Benzoic acid	122	C7H6O2	000065-85-0	94
4			Benzoic acid	122	C7H6O2	000065-85-0	91
5			Cyclobutane-1,1-dicarboxamide, N...	382	C20H18N2O6	1000253-25-3	91



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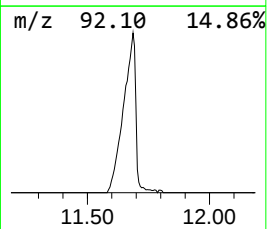
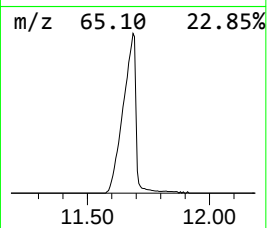
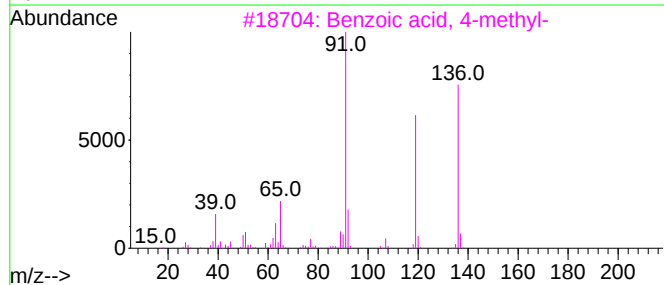
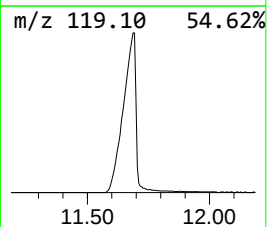
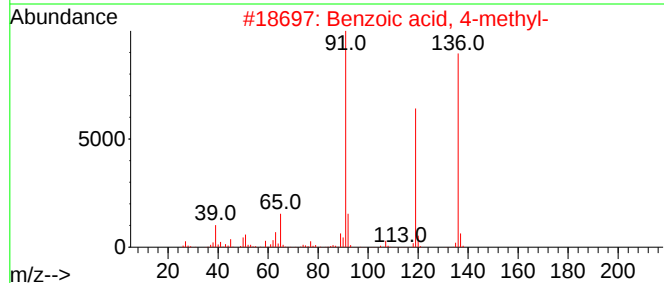
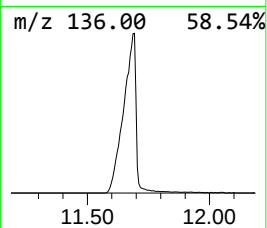
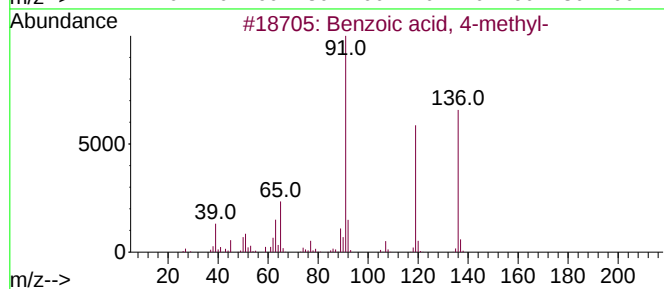
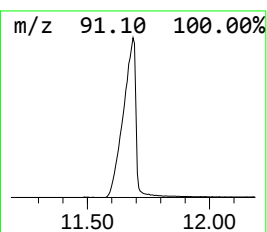
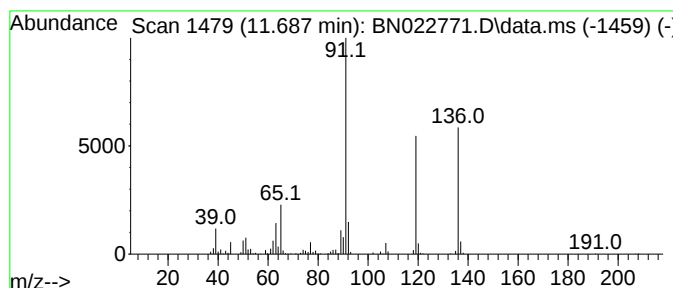
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Benzoic acid, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	43.05 ng/ul	1274730	Naphthalene-d8	10.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	96
2			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	96
3			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	96
4			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	94
5			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	94



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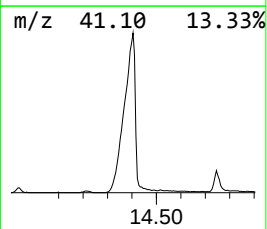
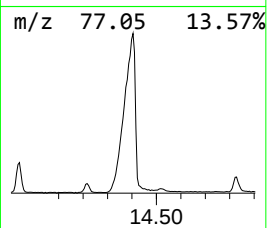
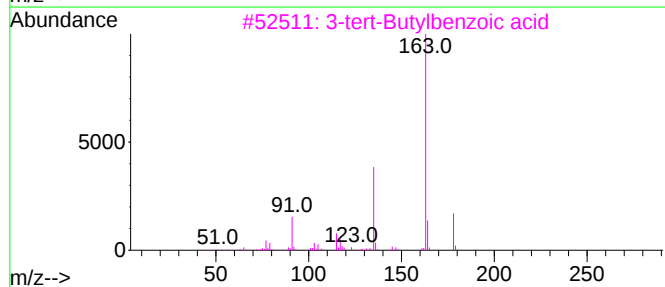
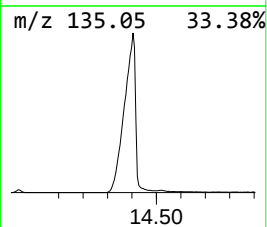
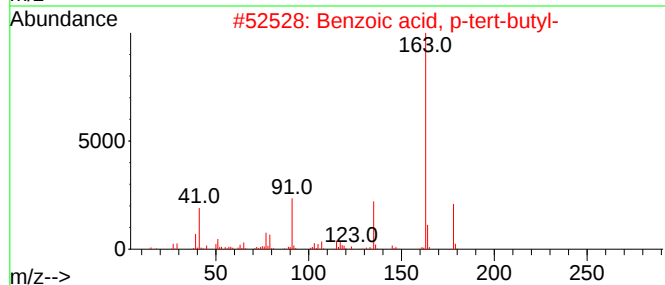
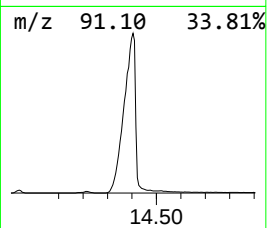
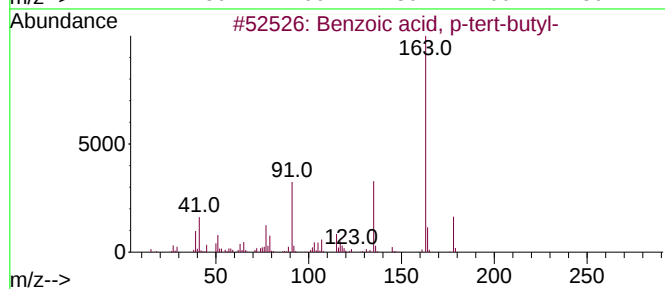
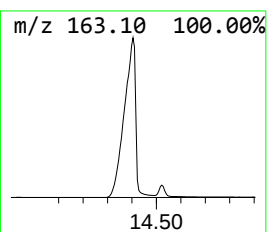
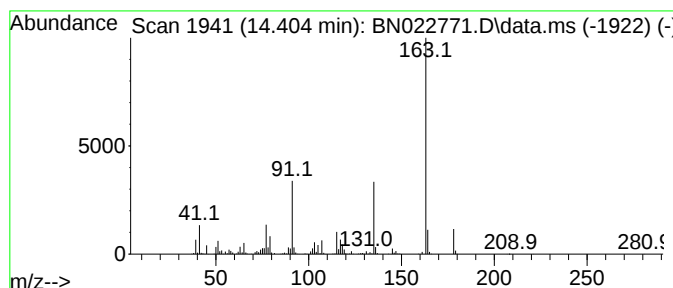
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Benzoic acid, p-tert-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.404	87.37 ng/ul	4005360	Acenaphthene-d10	14.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	96
2			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	93
3			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	87
4			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	76
5			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	76



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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
Hexanoic acid, ...	9.346	166.0	ng/ul	4915580	2	10.669	592188	20.0
Benzoic acid	10.087	60.3	ng/ul	1784600	2	10.669	592188	20.0
Benzoic acid, 4...	11.687	43.0	ng/ul	1274730	2	10.669	592188	20.0
Benzoic acid, p...	14.404	87.4	ng/ul	4005360	3	14.522	916892	20.0