LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
Acq On : 08 Mar 2023 21:45
Operator : CG/JU
Sample : 01729-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

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_P\Methods\SFAM-EPA-BP030723.M
Title : SVOA CALIBRATION

Signal : TIC: BP013989.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.228	4	7	21	rVB	132829	201249	3.98%	0.460%
2	3.434	38	42	57	rVB	25328	42465	0.84%	0.097%
3	3.728	89	92	101	rVB	7086	10368	0.20%	0.024%
4	3.875	114	117	135	rBV	127403	221611	4.38%	0.506%
5	4.099	149	155	163	rBV2	12929	21132	0.42%	0.048%
6	4.205	169	173	181	rBV2	8071	12547	0.25%	0.029%
7	4.305	187	190	194	rBV5	7103	9875	0.20%	0.023%
8	4.587	230	238	241	rBV8	2719	5304	0.10%	0.012%
9	5.140	327	332	337	rBV2	7711	12753	0.25%	0.029%
10	6.452	550	555	560	rBV5	6456	11824	0.23%	0.027%
11	7.234	682	688	699	rVB	81173	144817	2.86%	0.331%
12	7.399	710	716	728	rBV	338250	535459	10.58%	1.223%
13	7.611	744	752	761	rBV	342744	567861	11.23%	1.297%
14	8.081	824	832	842	rBV	432254	700298	13.84%	1.600%
15	8.787	943	952	964	rBV	272800	469162	9.27%	1.072%
16	9.252	1021	1031	1045	rBV	442608	746729	14.76%	1.706%
17	9.481	1045	1070	1090	rVV	826891	3611844	71.40%	8.250%
18	9.640	1094	1097	1102	rVB5	6380	10892	0.22%	0.025%
19	9.981	1146	1155	1167	rBV	391263	656664	12.98%	1.500%
20	10.158	1181	1185	1193	rBV	24039	58333	1.15%	0.133%
21	10.522	1237	1247	1261	rBV	603710	1022320	20.21%	2.335%
22	10.905	1301	1312	1320	rBV	598986	1001467	19.80%	2.288%
23	11.040	1326	1335	1353	rBV	497111	909023	17.97%	2.076%
24	11.175	1355	1358	1366	rVB9	3172	7355	0.15%	0.017%
25	11.322	1382	1383	1390	rVB7	3921	6523	0.13%	0.015%
26	11.728	1444	1452	1453	rBV6	9010	17998	0.36%	0.041%
27	11.846	1462	1472	1477	rBV8	7380	23666	0.47%	0.054%
28	11.987	1494	1496	1504	rVB8	3552	5144	0.10%	0.012%
29	12.481	1575	1580	1586	rBV	8857	15507	0.31%	0.035%
30	12.610	1597	1602	1611	rBV2	18623	31954	0.63%	0.073%
31	13.522	1754	1757	1763	rVB7	4247	5837	0.12%	0.013%
32	14.122	1851	1859	1873	rBV	1364257	1830747	36.19%	4.182%
33	14.234	1873	1878	1882	rVV8	4447	7703	0.15%	0.018%
34	14.416	1902	1909	1917	rVV	1249546	1854740	36.66%	4.237%
35	14.510	1920	1925	1935	rVV	85328	153019	3.02%	0.350%
36	14.593	1937	1939	1945	rVB6	7513	10375	0.21%	0.024%

LSC Area Percent Report

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Acq On : 08 Mar 2023 21:45
Operator : CG/JU
Sample : 01729-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

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_P\Methods\SFAM-EPA-BP030723.M
Title : SVOA CALIBRATION

37	14.716	1953	1960	1970	rVB	999076	1507680	29.80%	3.444%
38	14.916	1989	1994	2007	rBV	71937	161796	3.20%	0.370%
39	15.122	2026	2029	2039	rVB9	9224	20322	0.40%	0.046%
40	15.457	2081	2086	2091	rBV5	8302	18853	0.37%	0.043%
41	15.710	2122	2129	2143	rBV	1848309	2570085	50.80%	5.871%
42	15.828	2143	2149	2160	rVV	713618	1029356	20.35%	2.351%
43	15.951	2165	2170	2175	rVB2	9223	16334	0.32%	0.037%
44	16.075	2184	2191	2200	rBV	306097	418540	8.27%	0.956%
45	16.410	2244	2248	2250	rBV5	3814	5214	0.10%	0.012%
46	16.640	2283	2287	2293	rBV	19165	26594	0.53%	0.061%
47	16.857	2319	2324	2329	rBV8	7247	13840	0.27%	0.032%
48	17.145	2371	2373	2378	rVB6	4197	5295	0.10%	0.012%
49	17.210	2381	2384	2388	rVB6	5440	7252	0.14%	0.017%
50	17.263	2388	2393	2399	rBV4	13378	24830	0.49%	0.057%
51	17.469	2422	2428	2439	rBV	1426654	2033626	40.20%	4.645%
52	17.575	2439	2446	2453	rVV	2198098	3205951	63.37%	7.323%
53	17.657	2456	2460	2468	rVB8	19290	37634	0.74%	0.086%
54	17.739	2471	2474	2480	rVB4	6696	10748	0.21%	0.025%
55	18.116	2534	2538	2544	rVB9	15960	19383	0.38%	0.044%
56	18.210	2552	2554	2559	rBV6	4461	6283	0.12%	0.014%
57	18.328	2569	2574	2583	rBV	176020	261024	5.16%	0.596%
58	18.734	2639	2643	2647	rBV3	25823	30880	0.61%	0.071%
59	19.145	2711	2713	2716	rBV4	9218	9735	0.19%	0.022%
60	19.369	2747	2751	2757	rBV2	36632	50991	1.01%	0.116%
61	19.439	2758	2763	2773	rVV	40819	81866	1.62%	0.187%
62	19.551	2779	2782	2790	rBV3	60782	95869	1.90%	0.219%
63	19.792	2817	2823	2833	rBV	3285259	4293377	84.87%	9.807%
64	21.216	3061	3065	3076	rBV	284086	479573	9.48%	1.095%
65	21.545	3116	3121	3130	rBV	2000869	2757313	54.50%	6.298%
66	23.927	3518	3526	3537	rVB2	2361829	5058887	100.00%	11.555%
67	24.086	3546	3553	3565	rVB2	1375683	2901439	57.35%	6.627%
68	24.951	3694	3700	3710	rVB	733618	1664179	32.90%	3.801%

Sum of corrected areas: 43779314

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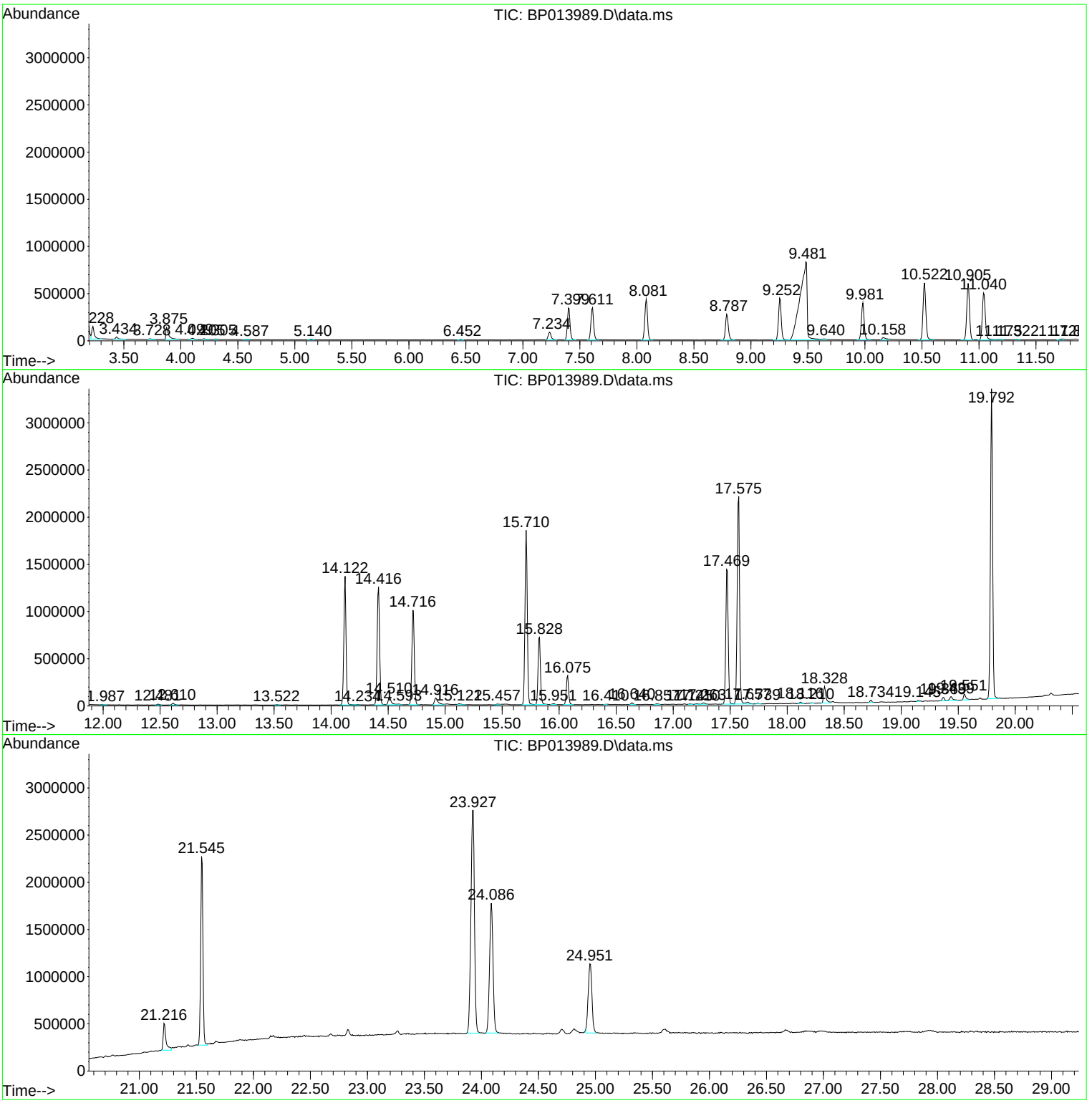
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
Acq On : 08 Mar 2023 21:45
Operator : CG/JU
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Quant Title : SVOA CALIBRATION

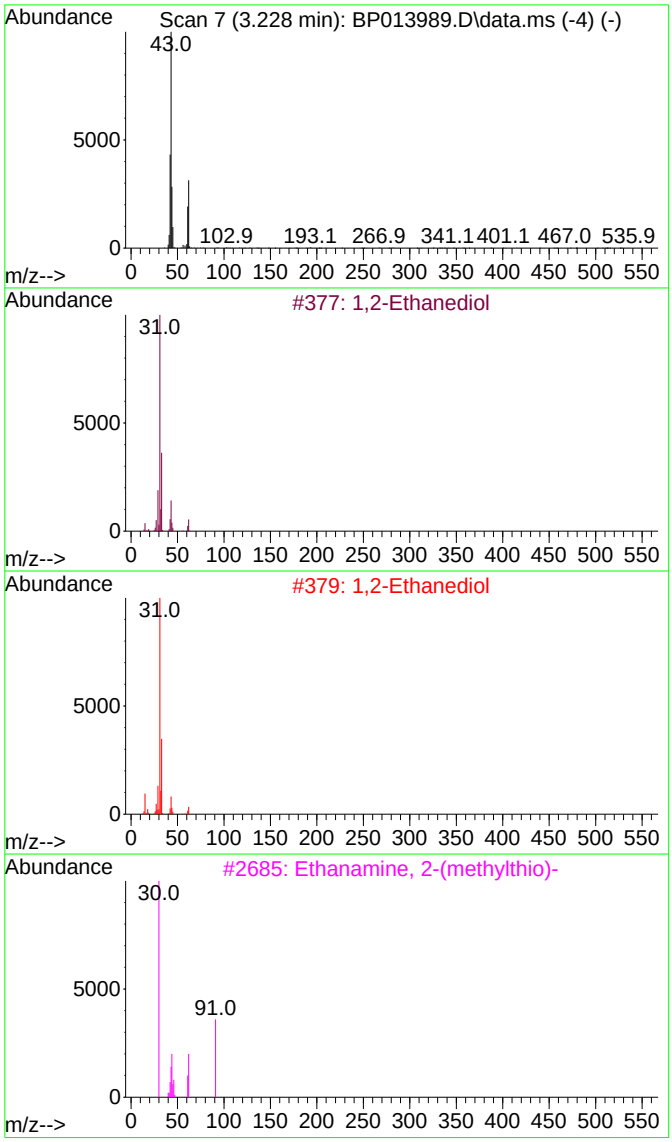
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

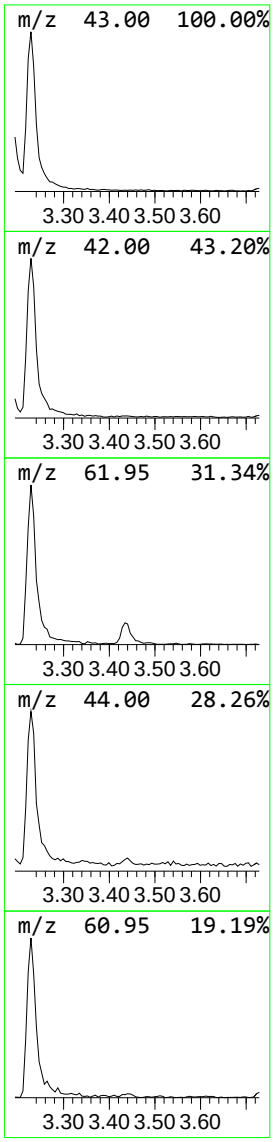
****

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.228	5.75 ng/ul	201249	1,4-Dichlorobenzene-d4	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol	62	C2H6O2	000107-21-1	9
2	1,2-Ethanediol	62	C2H6O2	000107-21-1	9
3	Ethanamine, 2-(methylthio)-	91	C3H9NS	018542-42-2	9
4	Ethanethiol	62	C2H6S	000075-08-1	4
5	Peroxide, dimethyl	62	C2H6O2	000690-02-8	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
Acq On : 08 Mar 2023 21:45
Operator : CG/JU
Sample : 01729-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

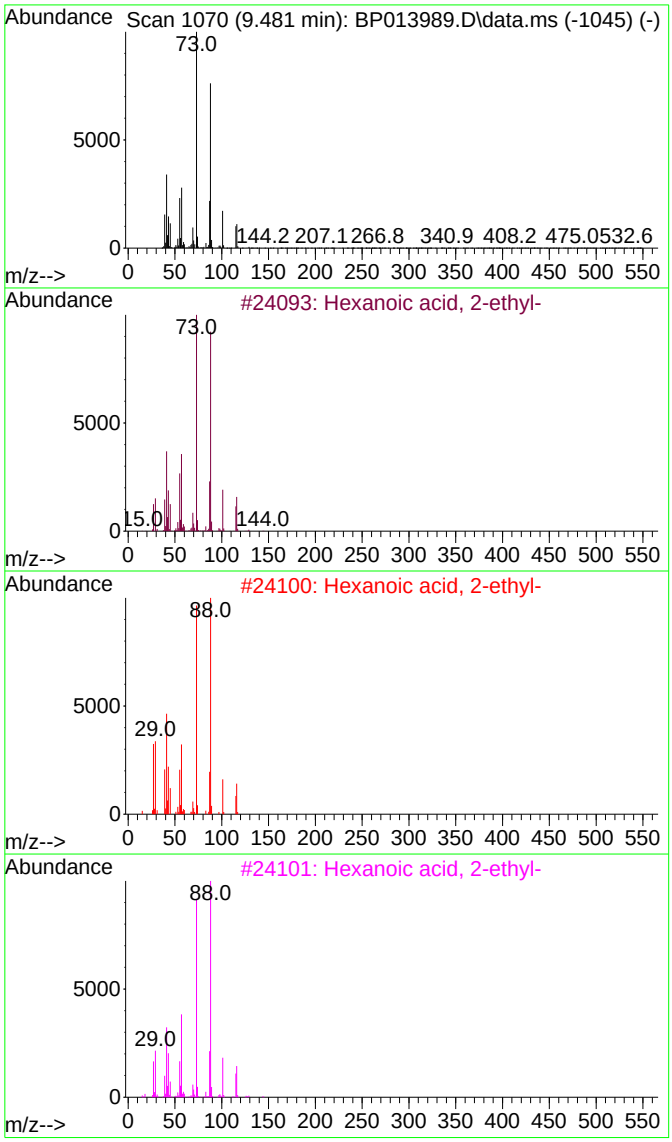
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

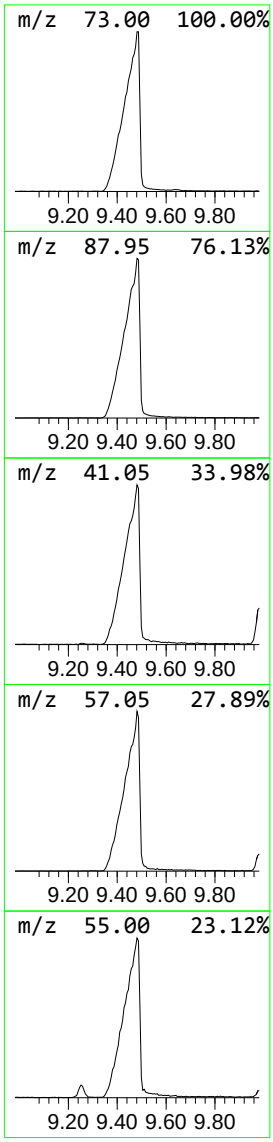
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.481	103.15 ng/ul	3611840	1,4-Dichlorobenzene-d4	8.081

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	90
3	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
4	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	83
5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
Acq On : 08 Mar 2023 21:45
Operator : CG/JU
Sample : 01729-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

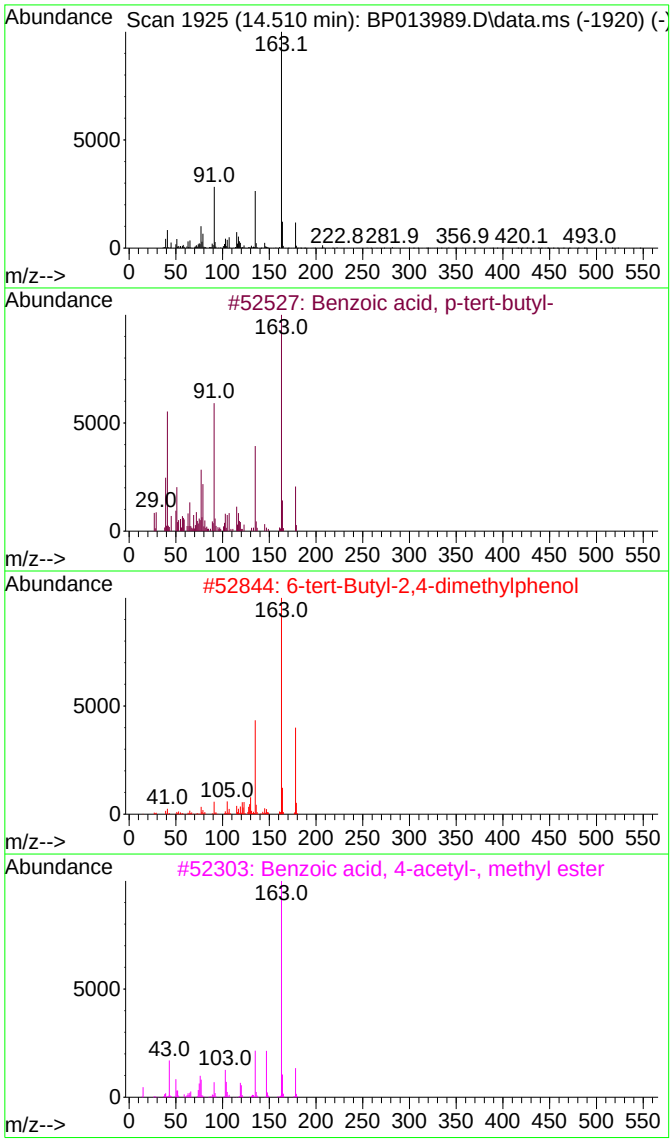
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

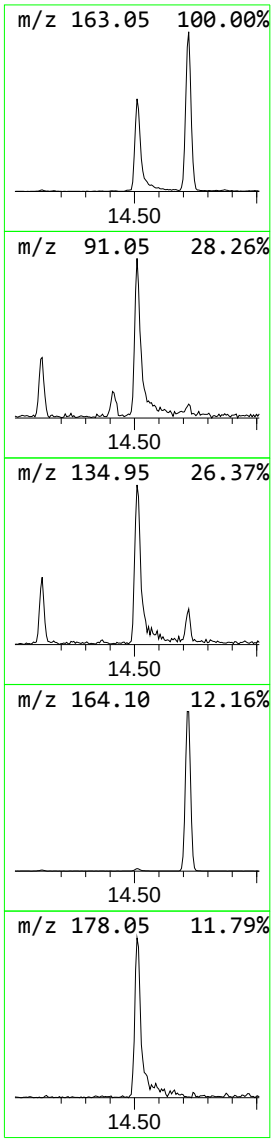
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzoic acid, p-tert-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	2.03 ng/ul	153019	Acenaphthene-d10	14.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	86
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	72
3	Benzoic acid, 4-acetyl-, methyl ...	178	C10H10O3	003609-53-8	72
4	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	70
5	Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
Acq On : 08 Mar 2023 21:45
Operator : CG/JU
Sample : 01729-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

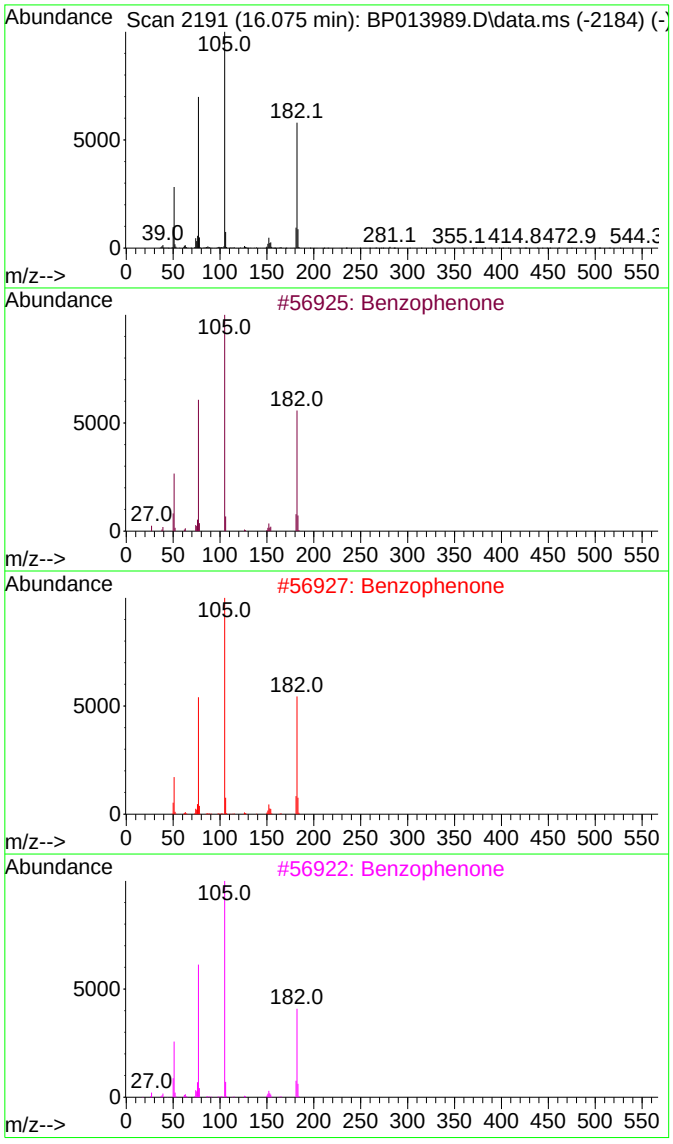
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

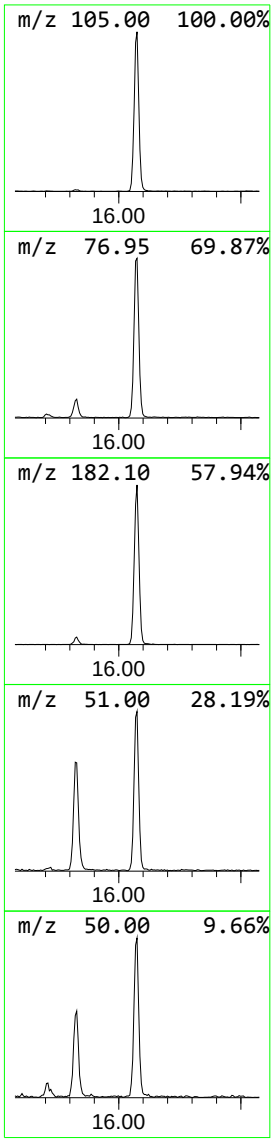
****

Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.075	5.55 ng/ul	418540	Acenaphthene-d10	14.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	91
5	1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	78





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

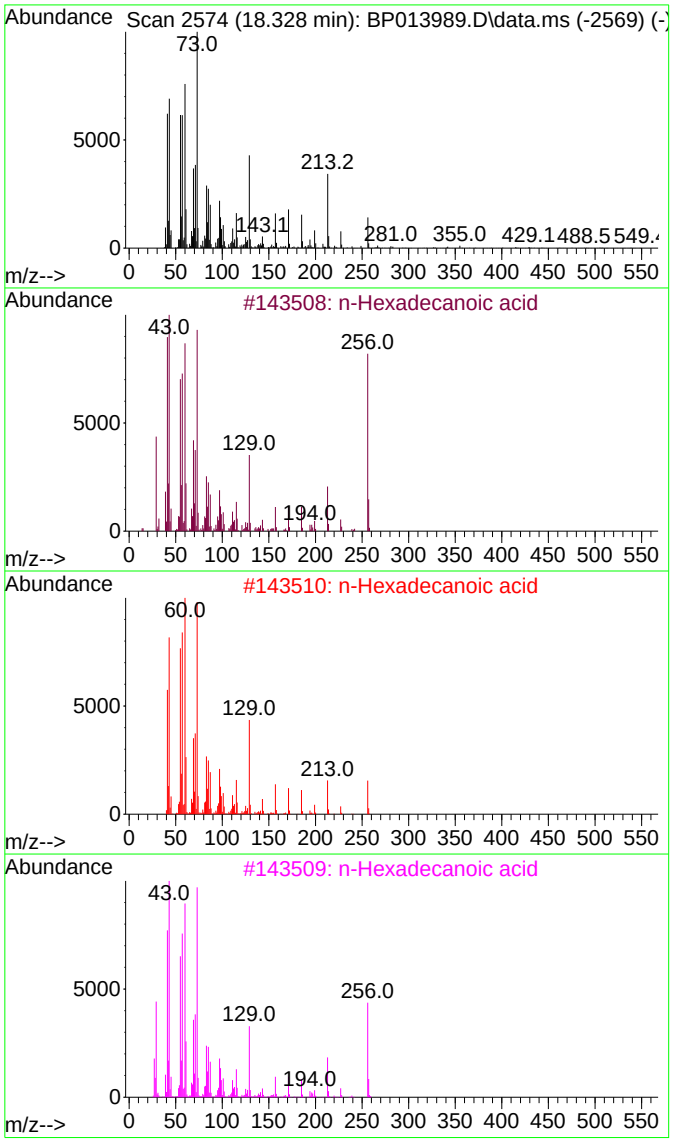
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

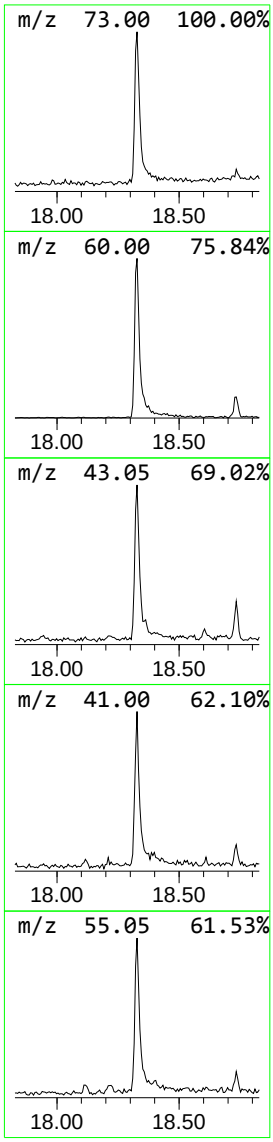
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.328	2.57 ng/ul	261024	Phenanthrene-d10	17.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

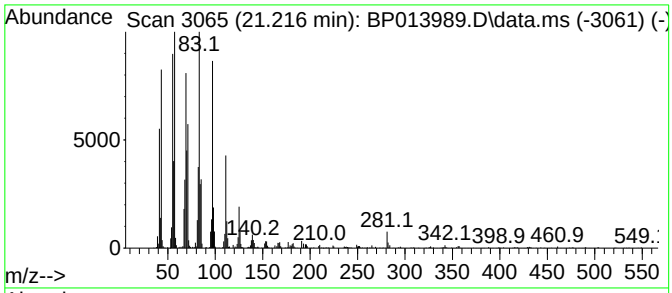
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

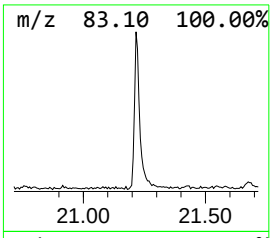
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

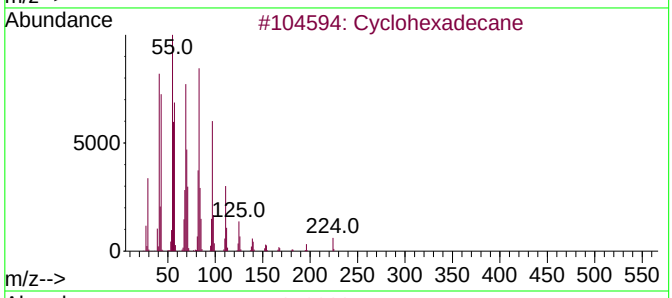
****
Peak Number 6 (DEL) Alkane: Cyclic21.216 Concentration Rank 5

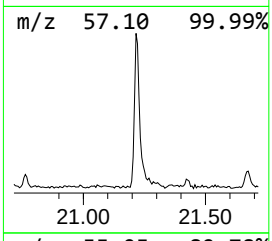
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.216	3.48 ng/ul	479573	Chrysene-d12	21.545

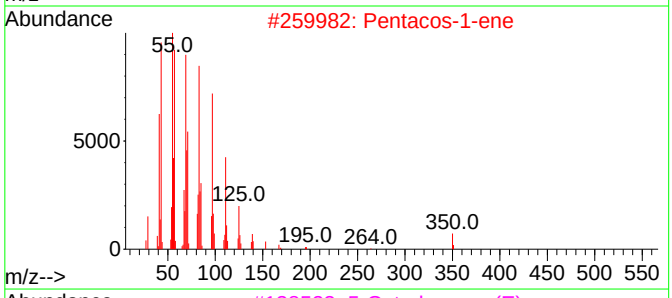
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	5-Octadecene, (E)-	252	C18H36	007206-21-5	93
4	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93

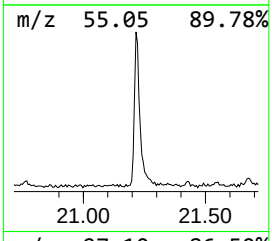


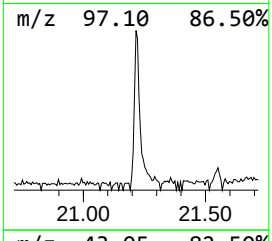


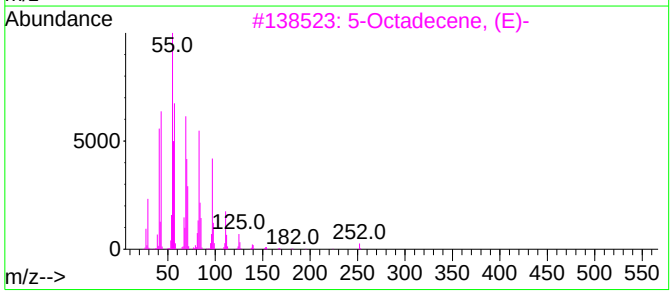


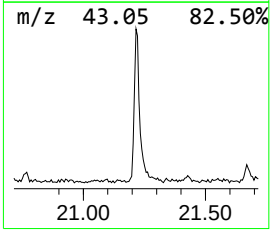












Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
Acq On : 08 Mar 2023 21:45
Operator : CG/JU
Sample : 01729-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

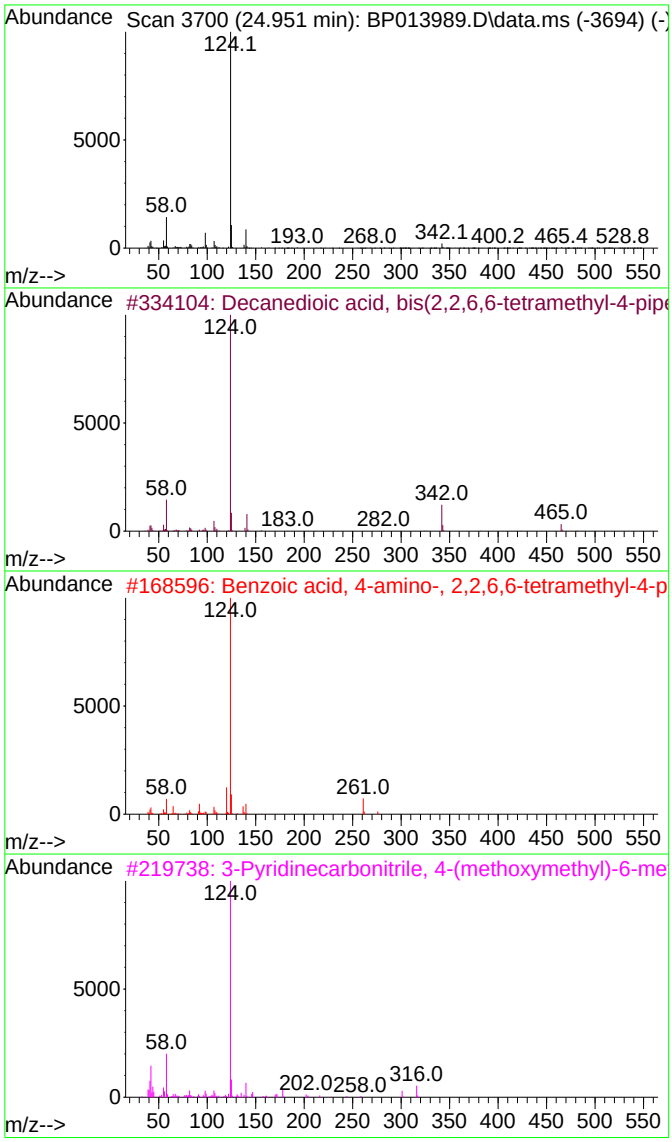
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

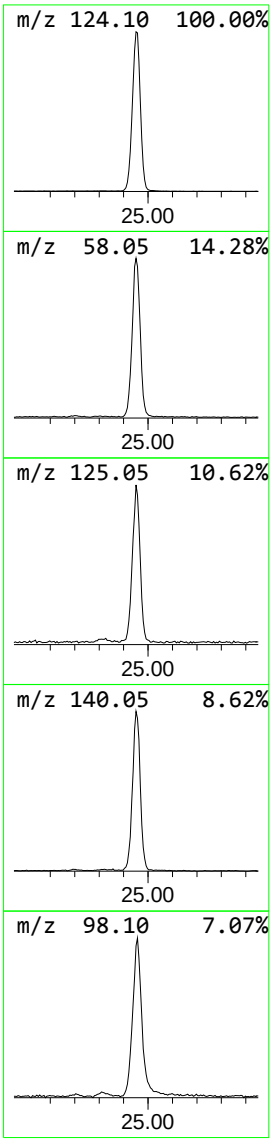
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Decanedioic acid, bis(2,2,6... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.951	11.47 ng/ul	1664180	Perylene-d12	24.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanedioic acid, bis(2,2,6,6-te...	480	C28H52N2O4	052829-07-9	72
2	Benzoic acid, 4-amino-, 2,2,6,6-...	276	C16H24N2O2	1000337-88-4	64
3	3-Pyridinecarbonitrile, 4-(metho...	316	C18H28N4O	1000320-13-0	64
4	N-Butyl-2,2,6,6-tetramethyl-4-pi...	358	C16H27F5N2O	1000470-17-2	64
5	8-Allyl-2-oxo-2H-chromene-3-carb...	368	C22H28N2O3	1000297-53-7	56





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030823\
Data File : BP013989.D
Acq On : 08 Mar 2023 21:45
Operator : CG/JU
Sample : 01729-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0BY8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP030723.M
Quant Title : SVOA CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	3.228	5.8	ng/ul	201249	1	8.081	700298	20.0
Hexanoic acid, ...	9.481	103.2	ng/ul	3611840	1	8.081	700298	20.0
Benzoic acid, p...	14.510	2.0	ng/ul	153019	3	14.716	1507680	20.0
Benzophenone	16.075	5.5	ng/ul	418540	3	14.716	1507680	20.0
n-Hexadecanoic ...	18.328	2.6	ng/ul	261024	4	17.469	2033630	20.0
(DEL) Alkane: C...	21.216	3.5	ng/ul	479573	5	21.545	2757310	20.0
Decanedioic aci...	24.951	11.5	ng/ul	1664180	6	24.086	2901440	20.0