LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
Data File : BF135697.D
Acq On : 10 Oct 2023 21:40
Operator : CG\JU
Sample : 04731-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DTP-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\Methods\8270-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135697.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.340	380	383	392	rBV2	37752	70653	3.47%	0.319%
2	4.963	484	489	506	rBV	1344067	1827777	89.76%	8.255%
3	5.375	556	559	587	rBV	1909115	2036233	100.00%	9.196%
4	5.763	621	625	629	rBV2	41765	43182	2.12%	0.195%
5	6.387	728	731	755	rBV	1891407	2018006	99.10%	9.114%
6	6.740	788	791	798	rBV	662832	587360	28.85%	2.653%
7	7.304	884	887	901	rBV	1428703	1299260	63.81%	5.868%
8	8.016	1005	1008	1019	rBV	837817	745705	36.62%	3.368%
9	9.092	1187	1191	1201	rBV	2118769	1875751	92.12%	8.471%
10	9.216	1208	1212	1217	rVB	31418	38811	1.91%	0.175%
11	9.775	1303	1307	1311	rBV	898574	765343	37.59%	3.457%
12	9.804	1311	1312	1319	rVB2	30557	33256	1.63%	0.150%
13	10.328	1399	1401	1406	rVB2	29456	29457	1.45%	0.133%
14	10.569	1438	1442	1457	rBV	1248864	1182294	58.06%	5.340%
15	10.880	1489	1495	1498	rBV3	19465	25112	1.23%	0.113%
16	11.169	1540	1544	1548	rVB2	25911	28783	1.41%	0.130%
17	11.269	1558	1561	1563	rBV	929389	753439	37.00%	3.403%
18	11.292	1563	1565	1571	rVV	519132	433285	21.28%	1.957%
19	11.351	1571	1575	1582	rVV	104378	113519	5.57%	0.513%
20	11.522	1598	1604	1608	rBV3	24365	33881	1.66%	0.153%
21	11.775	1645	1647	1650	rBV	73620	61002	3.00%	0.276%
22	11.804	1650	1652	1658	rVV	192135	190696	9.37%	0.861%
23	11.857	1658	1661	1663	rVV2	40058	42419	2.08%	0.192%
24	11.886	1663	1666	1669	rVV	127215	133687	6.57%	0.604%
25	11.910	1669	1670	1674	rVB	49731	34451	1.69%	0.156%
26	12.075	1695	1698	1702	rVB	48702	45452	2.23%	0.205%
27	12.327	1738	1741	1744	rBV	51490	48931	2.40%	0.221%
28	12.369	1744	1748	1753	rVB4	37265	58580	2.88%	0.265%
29	12.427	1753	1758	1761	rBV2	27089	36628	1.80%	0.165%
30	12.492	1765	1769	1773	rBV	885325	768662	37.75%	3.471%
31	12.592	1783	1786	1791	rBV2	23358	25496	1.25%	0.115%
32	12.645	1792	1795	1798	rVV2	32369	26764	1.31%	0.121%
33	12.722	1802	1808	1813	rVV	689244	719065	35.31%	3.247%
34	12.774	1813	1817	1822	rVB4	30803	48694	2.39%	0.220%
35	12.863	1826	1832	1836	rBV	1652045	1443010	70.87%	6.517%
36	12.939	1842	1845	1851	rBV4	42666	76610	3.76%	0.346%

LSC Area Percent Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DTP-3

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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_F\Methods\8270-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.033	1857	1861	1862	rBV4	32607	41409	2.03%	0.187%
38	13.057	1862	1865	1869	rVV	94166	88978	4.37%	0.402%
39	13.122	1873	1876	1879	rVV	72880	58735	2.88%	0.265%
40	13.163	1879	1883	1890	rVB3	58927	83401	4.10%	0.377%
41	13.251	1895	1898	1901	rBV	30758	30279	1.49%	0.137%
42	13.286	1901	1904	1907	rBV2	33222	27816	1.37%	0.126%
43	13.439	1926	1930	1932	rBV3	36737	39153	1.92%	0.177%
44	13.580	1951	1954	1960	rVB	36787	41342	2.03%	0.187%
45	13.680	1966	1971	1973	rBV	55896	64144	3.15%	0.290%
46	13.704	1973	1975	1978	rVV	50371	45589	2.24%	0.206%
47	13.733	1978	1980	1982	rVV	44721	39559	1.94%	0.179%
48	13.769	1982	1986	1988	rVV4	35056	49370	2.42%	0.223%
49	13.792	1988	1990	1995	rVB	45255	40975	2.01%	0.185%
50	13.857	1995	2001	2004	rBV3	30535	62783	3.08%	0.284%
51	13.927	2007	2013	2016	rVV2	584005	843637	41.43%	3.810%
52	13.957	2016	2018	2025	rVV	289419	298058	14.64%	1.346%
53	14.039	2029	2032	2037	rVB	59909	56997	2.80%	0.257%
54	14.092	2037	2041	2045	rBV5	41452	66599	3.27%	0.301%
55	14.327	2076	2081	2084	rBV	61552	73061	3.59%	0.330%
56	14.357	2084	2086	2089	rVV	28981	24898	1.22%	0.112%
57	14.398	2089	2093	2096	rVV4	42258	53916	2.65%	0.243%
58	14.451	2100	2102	2104	rVV	36316	35536	1.75%	0.160%
59	14.474	2104	2106	2108	rVB	31678	25751	1.26%	0.116%
60	14.663	2133	2138	2142	rBV6	21709	45683	2.24%	0.206%
61	14.827	2163	2166	2169	rBV3	34018	37736	1.85%	0.170%
62	14.974	2187	2191	2195	rBV	261966	403156	19.80%	1.821%
63	15.033	2199	2201	2207	rVB4	33403	41462	2.04%	0.187%
64	15.092	2207	2211	2215	rBV	48234	61568	3.02%	0.278%
65	15.221	2231	2233	2238	rVB3	18040	20982	1.03%	0.095%
66	15.280	2239	2243	2249	rVB	171128	204835	10.06%	0.925%
67	15.345	2250	2254	2260	rBV	229432	282998	13.90%	1.278%
68	15.404	2260	2264	2268	rBV	391662	503101	24.71%	2.272%
69	15.586	2292	2295	2299	rBV5	16173	21894	1.08%	0.099%
70	15.633	2299	2303	2309	rVB4	17633	35265	1.73%	0.159%
71	15.845	2335	2339	2344	rBV6	18091	37396	1.84%	0.169%
72	15.974	2356	2361	2367	rBV5	18860	36350	1.79%	0.164%
73	16.904	2512	2519	2528	rBV2	99878	223337	10.97%	1.009%
74	17.080	2545	2549	2554	rBV3	20441	33798	1.66%	0.153%
75	17.139	2555	2559	2566	rVB3	24350	52839	2.59%	0.239%
76	17.357	2591	2596	2604	rVB	75453	159596	7.84%	0.721%

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DTP-3

Integration Parameters: rteint.p
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	17.633	2637	2643	2650	rVB3	20105	46879	2.30%	0.212%

Sum of corrected areas: 22142115

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Sample : 04731-07
Misc :
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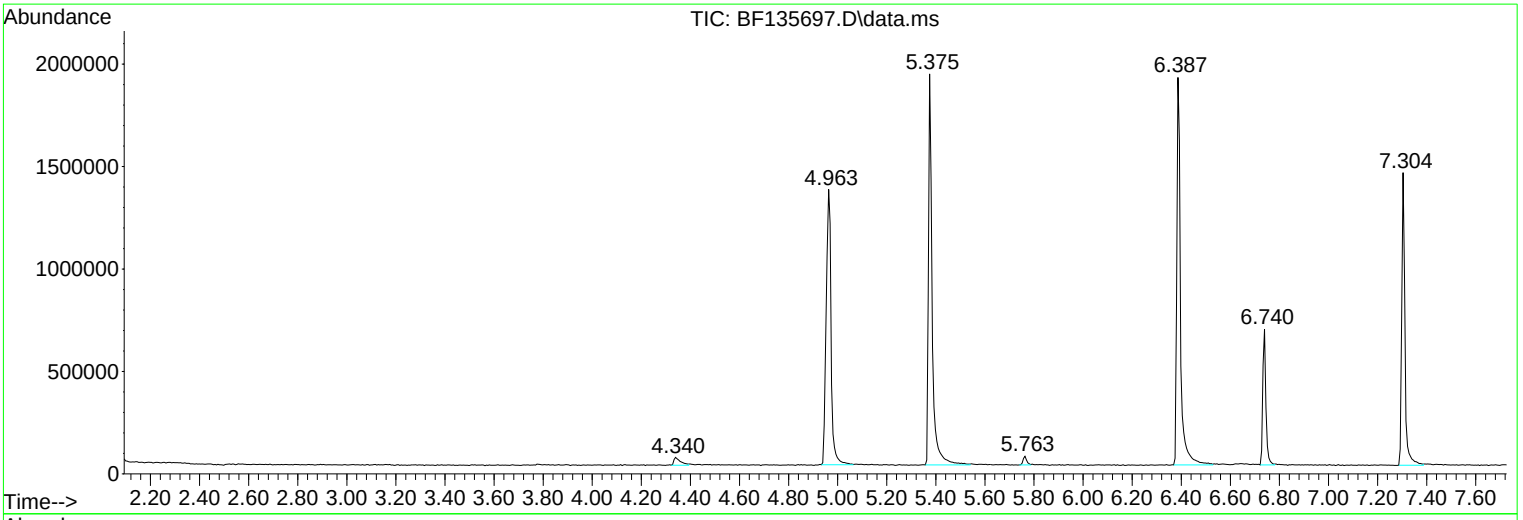
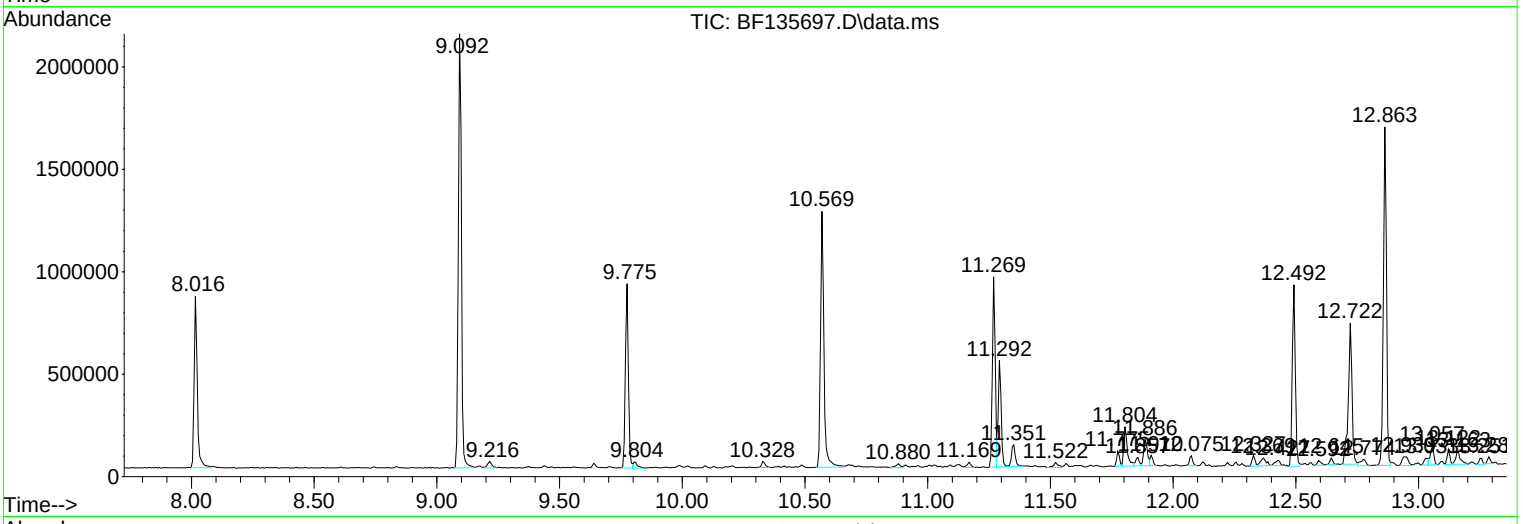
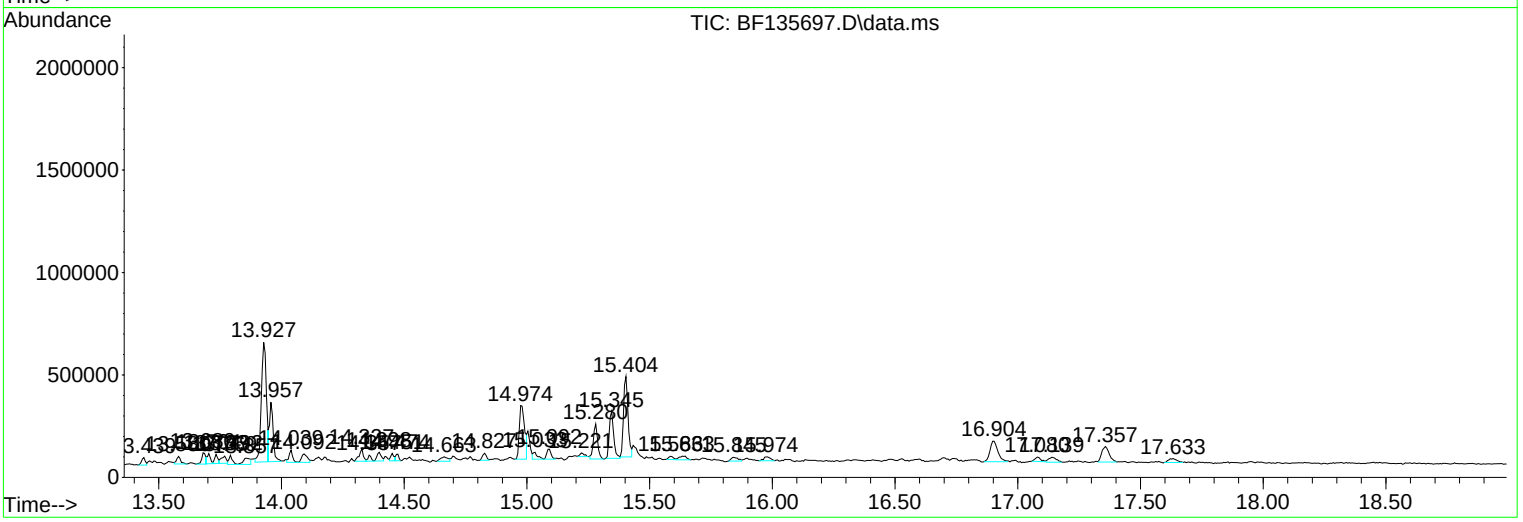
Instrument :
BNA_F
ClientSampleId :
DTP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	2.41 ng	70653	1,4-Dichlorobenzene-d4	6.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	64

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	62.24 ng	1827780	1,4-Dichlorobenzene-d4	6.740

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9

****

Peak Number 3 Phenanthrene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	5.06 ng	190696	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
2	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	92
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	91

****

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	3.55 ng	133687	Phenanthrene-d10	11.269

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DTP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	89
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	40
4	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	38
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	25

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Peak Number 5 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.057	2.11 ng	88978	Chrysene-d12	13.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	83
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64

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Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.45 ng	61568	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	94
2	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	91
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90

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Peak Number 7 Perylene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	8.14 ng	204835	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	97
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	96
4	Perylene	252	C20H12	000198-55-0	95
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	95

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 8 Picene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	2.10 ng	52839	Perylene-d12	15.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Picene	278	C22H14	000213-46-7	58
2	Benzo[b]triphenylene	278	C22H14	000215-58-7	58
3	Benzo[b]chrysene	278	C22H14	000214-17-5	58
4	Pentaphene	278	C22H14	000222-93-5	58
5	Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	53

Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
3-Penten-2-one,...	4.340	2.4	ng	70653	1	6.740	587360	20.0
2-Pentanone, 4-...	4.963	62.2	ng	1827780	1	6.740	587360	20.0
Phenanthrene, 1...	11.804	5.1	ng	190696	4	11.269	753439	20.0
4H-Cyclopenta[d...	11.886	3.5	ng	133687	4	11.269	753439	20.0
Pyrene, 1-methyl-	13.057	2.1	ng	88978	5	13.933	843637	20.0
Benzo[e]pyrene	15.092	2.5	ng	61568	6	15.404	503101	20.0
Perylene	15.280	8.1	ng	204835	6	15.404	503101	20.0
Picene	17.139	2.1	ng	52839	6	15.404	503101	20.0