

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101023\
 Data File : BF135699.D
 Acq On : 10 Oct 2023 22:41
 Operator : CG\JU
 Sample : 04800-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EO-01-100623

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: BF135699.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	485	488	500	rVB	341744	461850	23.94%	2.700%
2	5.375	556	559	580	rBV	1754319	1929364	100.00%	11.279%
3	5.763	616	625	631	rBV4	16087	30399	1.58%	0.178%
4	5.981	656	662	668	rVB5	13002	21435	1.11%	0.125%
5	6.387	728	731	742	rBV	1851494	1882631	97.58%	11.006%
6	6.569	758	762	767	rBV2	80769	72585	3.76%	0.424%
7	6.740	788	791	797	rBV	726314	627676	32.53%	3.669%
8	6.875	811	814	818	rBV2	22204	23569	1.22%	0.138%
9	7.010	830	837	840	rBV4	29842	44363	2.30%	0.259%
10	7.069	843	847	852	rVB2	27774	39563	2.05%	0.231%
11	7.122	852	856	859	rBV2	36233	41073	2.13%	0.240%
12	7.269	875	881	884	rBV2	35315	36913	1.91%	0.216%
13	7.304	884	887	890	rBV	1397330	1184585	61.40%	6.925%
14	7.328	890	891	895	rVB	178969	110799	5.74%	0.648%
15	7.534	923	926	930	rVB	50494	44584	2.31%	0.261%
16	7.628	937	942	943	rBV3	22579	26819	1.39%	0.157%
17	7.645	943	945	948	rVV3	23367	22981	1.19%	0.134%
18	7.692	951	953	957	rVB2	33157	33076	1.71%	0.193%
19	7.734	957	960	961	rBV	19377	19519	1.01%	0.114%
20	7.763	961	965	967	rVB4	31548	39623	2.05%	0.232%
21	7.998	1001	1005	1006	rBV	163539	152867	7.92%	0.894%
22	8.016	1006	1008	1014	rVV	922974	803735	41.66%	4.699%
23	8.075	1014	1018	1021	rVV2	57240	71965	3.73%	0.421%
24	8.104	1021	1023	1026	rVB2	23498	19382	1.00%	0.113%
25	8.186	1031	1037	1039	rBV6	15631	29042	1.51%	0.170%
26	8.210	1039	1041	1044	rVB2	35991	32551	1.69%	0.190%
27	8.304	1053	1057	1064	rVB5	40412	64494	3.34%	0.377%
28	8.357	1064	1066	1070	rBV4	20494	24078	1.25%	0.141%
29	8.392	1070	1072	1076	rVB3	38940	39038	2.02%	0.228%
30	8.434	1076	1079	1081	rBV	65007	56407	2.92%	0.330%
31	8.522	1090	1094	1096	rBV2	62200	56304	2.92%	0.329%
32	8.604	1105	1108	1112	rBV	185600	161015	8.35%	0.941%
33	8.675	1117	1120	1123	rVV3	44127	60653	3.14%	0.355%
34	8.704	1123	1125	1128	rVB3	30538	27561	1.43%	0.161%
35	8.839	1145	1148	1150	rBV3	62045	51905	2.69%	0.303%
36	8.886	1154	1156	1158	rBV2	24622	21233	1.10%	0.124%

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Stop Thrs : 0

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37	8.969	1166	1170	1174	rBV4	32733	45746	2.37%	0.267%
38	9.033	1179	1181	1183	rBV2	52739	41410	2.15%	0.242%
39	9.092	1188	1191	1195	rBV	1916081	1766311	91.55%	10.326%
40	9.175	1200	1205	1209	rVV	181383	161873	8.39%	0.946%
41	9.216	1209	1212	1214	rVV2	37204	39665	2.06%	0.232%
42	9.245	1214	1217	1220	rVB3	30230	31116	1.61%	0.182%
43	9.369	1235	1238	1241	rVB4	24040	28461	1.48%	0.166%
44	9.433	1246	1249	1251	rVV3	38360	52566	2.72%	0.307%
45	9.492	1255	1259	1261	rVV3	73332	86268	4.47%	0.504%
46	9.516	1261	1263	1266	rVV2	38431	41772	2.17%	0.244%
47	9.551	1266	1269	1272	rVB2	39556	36277	1.88%	0.212%
48	9.633	1279	1283	1287	rBV6	16937	30569	1.58%	0.179%
49	9.704	1292	1295	1299	rBV	189387	141562	7.34%	0.828%
50	9.745	1299	1302	1303	rBV2	19296	19633	1.02%	0.115%
51	9.775	1303	1307	1311	rVV	964765	787279	40.81%	4.602%
52	9.880	1322	1325	1330	rVB5	20040	23102	1.20%	0.135%
53	9.933	1330	1334	1337	rBV4	23814	38793	2.01%	0.227%
54	10.028	1346	1350	1353	rBV3	47131	50765	2.63%	0.297%
55	10.098	1358	1362	1365	rBV4	19085	24362	1.26%	0.142%
56	10.204	1377	1380	1383	rVB	167789	132288	6.86%	0.773%
57	10.333	1400	1402	1409	rVB7	15679	22611	1.17%	0.132%
58	10.428	1413	1418	1424	rVB	58606	75118	3.89%	0.439%
59	10.569	1439	1442	1453	rVB	1143098	1074344	55.68%	6.281%
60	10.680	1458	1461	1470	rVB	161954	195655	10.14%	1.144%
61	10.869	1491	1493	1498	rBV4	15436	30106	1.56%	0.176%
62	10.904	1498	1499	1502	rVB2	26721	21146	1.10%	0.124%
63	11.127	1534	1537	1540	rBV	100519	94607	4.90%	0.553%
64	11.157	1540	1542	1548	rVB2	58293	64325	3.33%	0.376%
65	11.269	1558	1561	1564	rBV	857722	730599	37.87%	4.271%
66	11.292	1564	1565	1571	rVB	66463	60629	3.14%	0.354%
67	11.510	1598	1602	1605	rBV5	19051	25643	1.33%	0.150%
68	11.557	1608	1610	1614	rVB	80562	73097	3.79%	0.427%
69	11.804	1649	1652	1656	rVV2	72161	79692	4.13%	0.466%
70	11.886	1664	1666	1669	rBV2	24031	21143	1.10%	0.124%
71	11.969	1677	1680	1683	rBV	72567	60059	3.11%	0.351%
72	12.327	1738	1741	1744	rBV4	19947	22830	1.18%	0.133%
73	12.357	1744	1746	1750	rVV2	45399	43142	2.24%	0.252%
74	12.492	1766	1769	1773	rBV	58740	64457	3.34%	0.377%
75	12.727	1804	1809	1813	rBV2	72245	100924	5.23%	0.590%
76	12.863	1828	1832	1839	rVB	1398268	1157967	60.02%	6.769%

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Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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77	13.092	1869	1871	1875	rBV2	25986	28784	1.49%	0.168%
78	13.439	1926	1930	1932	rBV	30535	34536	1.79%	0.202%
79	13.768	1983	1986	1990	rBV3	23867	27323	1.42%	0.160%
80	13.933	2010	2014	2018	rBV	507017	495275	25.67%	2.895%
81	14.086	2038	2040	2043	rBV2	23803	22029	1.14%	0.129%
82	14.392	2090	2092	2096	rBV3	32712	36771	1.91%	0.215%
83	15.404	2260	2264	2269	rBV	413902	497539	25.79%	2.909%

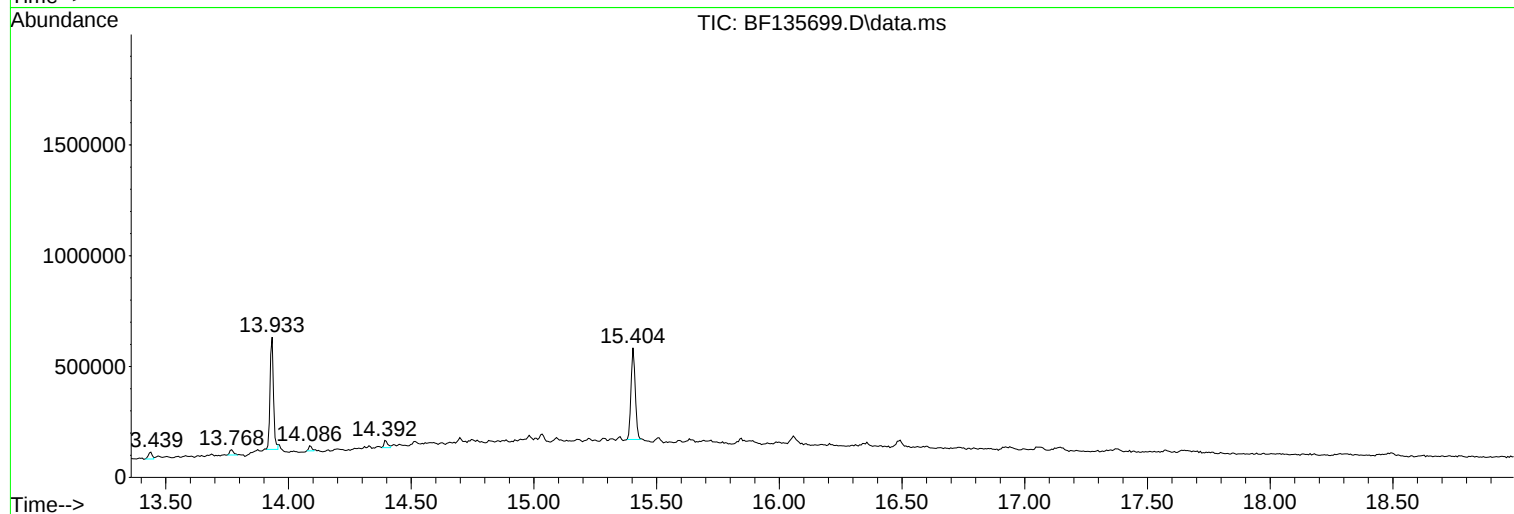
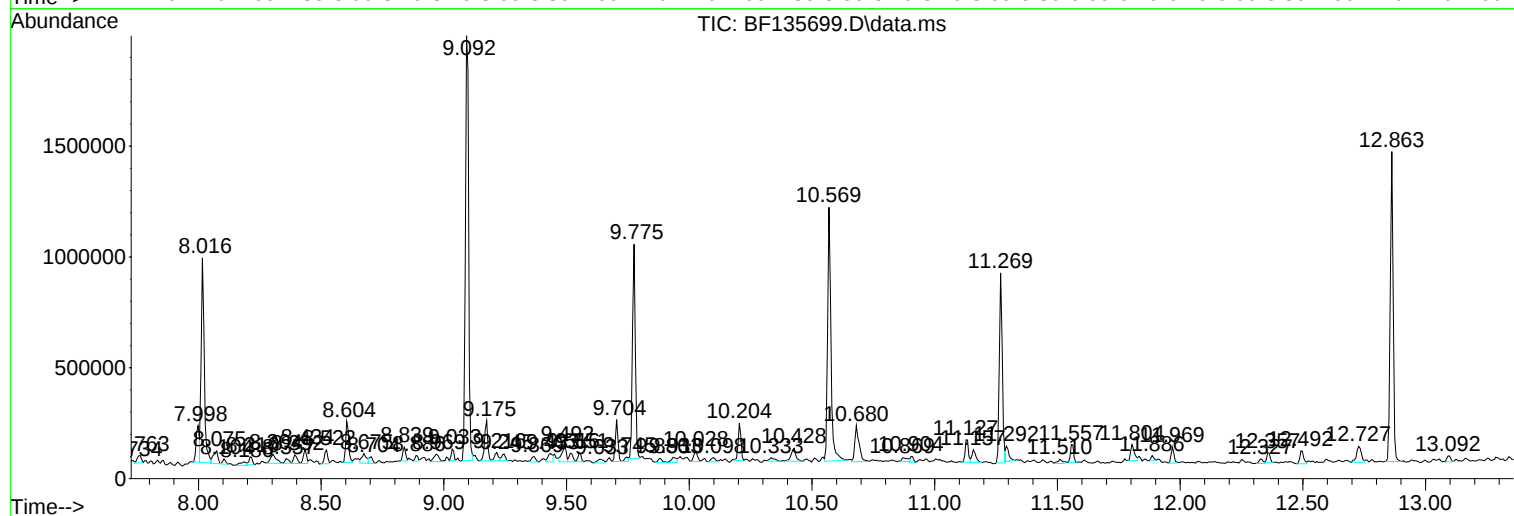
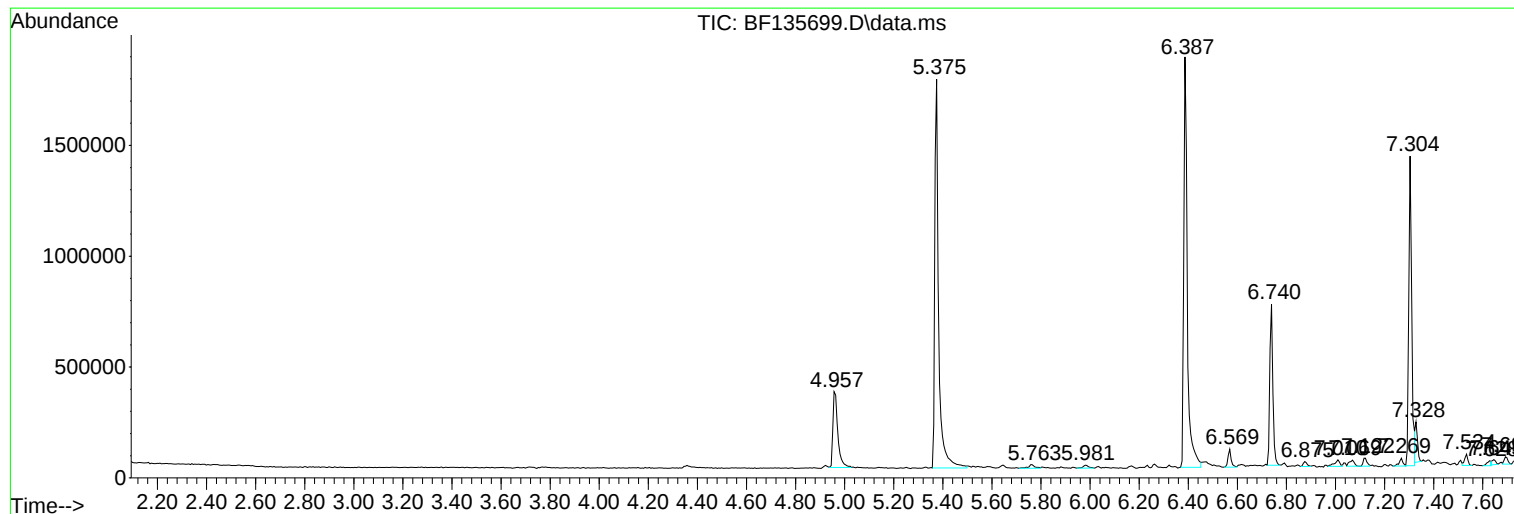
Sum of corrected areas: 17105806

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



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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.957	14.72 ng	461850	1,4-Dichlorobenzene-d4	6.739	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10

Peak Number 2 Oxalic acid, isobutyl nonyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.569	2.31 ng	72585	1,4-Dichlorobenzene-d4	6.739	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	80
2	Tetradecane	198	C14H30	000629-59-4	78
3	Nonane, 2-methyl-	142	C10H22	000871-83-0	72
4	Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	64
5	Hexadecane	226	C16H34	000544-76-3	59

Peak Number 3 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
8.604	4.01 ng	161015	Naphthalene-d8		8.016	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	90
2	Hexadecane		226	C16H34	000544-76-3	90
3	Silane, trichlorooctadecyl-		386	C18H37Cl3Si	000112-04-9	90
4	Heptadecane		240	C17H36	000629-78-7	86
5	Tridecane		184	C13H28	000629-50-5	78

Peak Number 4 Tetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.175	4.11 ng	161873	Acenaphthene-d10	9.775

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	95
2	Hexadecane	226	C16H34	000544-76-3	90
3	Nonadecane	268	C19H40	000629-92-5	86
4	Tridecane	184	C13H28	000629-50-5	86
5	Undecane	156	C11H24	001120-21-4	86

Peak Number 5 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.492	2.19 ng	86268	Acenaphthene-d10	9.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	80
2	3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	64
3	Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	59
4	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	59
5	Nonane, 5-(2-methylpropyl)-	184	C13H28	062185-53-9	53

Peak Number 6 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.704	3.60 ng	141562	Acenaphthene-d10	9.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tetradecane	198	C14H30	000629-59-4	90
4	Tridecane, 4,8-dimethyl-	212	C15H32	055030-62-1	86
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86

Peak Number 7 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	3.36 ng	132288	Acenaphthene-d10	9.775

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Nonadecane	268	C19H40	000629-92-5	87
3	Eicosane	282	C20H42	000112-95-8	86
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	83

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TIC Library : C:\Database\NIST0.L
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Peak Number 8 Eicosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.680	5.36 ng	195655	Phenanthrene-d10	11.269

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90	
2	Eicosane	282	C20H42	000112-95-8	90	
3	Tridecane	184	C13H28	000629-50-5	87	
4	Nonadecane	268	C19H40	000629-92-5	87	
5	Pentadecane	212	C15H32	000629-62-9	83	

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.128	2.59 ng	94607	Phenanthrene-d10	11.269

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91	
2	Tetracosane	338	C24H50	000646-31-1	90	
3	Octacosane	394	C28H58	000630-02-4	86	
4	Nonadecane	268	C19H40	000629-92-5	86	
5	Heneicosane	296	C21H44	000629-94-7	86	

Peak Number 10 Tetradecane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.557	2.00 ng	73097	Phenanthrene-d10	11.269

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90	
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86	
3	Hexadecane	226	C16H34	000544-76-3	86	
4	Nonadecane	268	C19H40	000629-92-5	83	
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	80	

Peak Number 11 n-Decanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

11.804 2.18 ng 79692 Phenanthrene-d10 11.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	50
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	46
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	38
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	25
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	25

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	14.7	ng	461850	1	6.739	627676	20.0
Oxalic acid, is...	6.569	2.3	ng	72585	1	6.739	627676	20.0
Nonadecane	8.604	4.0	ng	161015	2	8.016	803735	20.0
Tetradecane	9.175	4.1	ng	161873	3	9.775	787279	20.0
Tetratetracontane	9.492	2.2	ng	86268	3	9.775	787279	20.0
Pentadecane	9.704	3.6	ng	141562	3	9.775	787279	20.0
Hexadecane	10.204	3.4	ng	132288	3	9.775	787279	20.0
Eicosane	10.680	5.4	ng	195655	4	11.269	730599	20.0
Tetracosane	11.128	2.6	ng	94607	4	11.269	730599	20.0
Tetradecane, 1-...	11.557	2.0	ng	73097	4	11.269	730599	20.0
n-Decanoic acid	11.804	2.2	ng	79692	4	11.269	730599	20.0