LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

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:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.898	473	478	488	rBV	332864	402804	18.33%	1.718%
2	5.322	545	550	554	rBV	2181610	2196936	100.00%	9.369%
3	6.351	720	725	728	rVB	2225167	2182360	99.34%	9.307%
4	6.481	743	747	750	rBV	2430890	2171986	98.86%	9.262%
5	6.710	782	786	790	rBV	853552	679084	30.91%	2.896%
6	6.869	809	813	816	rVB	1776869	1505436	68.52%	6.420%
7	7.269	876	881	884	rBV	1362305	1330223	60.55%	5.673%
8	7.375	893	899	904	rVB	36002	40486	1.84%	0.173%
9	7.992	1000	1004	1007	rBV	1030710	840174	38.24%	3.583%
10	9.075	1183	1188	1197	rBV	1920418	1766669	80.42%	7.534%
11	9.463	1251	1254	1257	rBV	474953	381027	17.34%	1.625%
12	9.604	1275	1278	1281	rVB	40780	31257	1.42%	0.133%
13	9.745	1298	1302	1306	rBV2	889056	773711	35.22%	3.299%
14	9.775	1306	1307	1310	rVB	32635	24034	1.09%	0.102%
15	9.951	1334	1337	1340	rVB	30362	25200	1.15%	0.107%
16	10.192	1375	1378	1382	rVB2	38071	31973	1.46%	0.136%
17	10.292	1392	1395	1399	rVB	37739	30603	1.39%	0.131%
18	10.533	1431	1436	1439	rBV	1061232	985626	44.86%	4.203%
19	10.663	1455	1458	1466	rBV	43064	52305	2.38%	0.223%
20	11.027	1517	1520	1525	rVB	25336	27186	1.24%	0.116%
21	11.116	1532	1535	1538	rBV2	29581	32199	1.47%	0.137%
22	11.227	1550	1554	1556	rBV	708511	609526	27.74%	2.599%
23	11.251	1556	1558	1561	rVV	415855	315441	14.36%	1.345%
24	11.298	1561	1566	1569	rVB	95977	85800	3.91%	0.366%
25	11.463	1586	1594	1602	rBV3	58757	95268	4.34%	0.406%
26	11.633	1618	1623	1628	rVB3	27403	31790	1.45%	0.136%
27	11.727	1633	1639	1641	rVV	62309	55915	2.55%	0.238%
28	11.757	1641	1644	1648	rVV	79006	73067	3.33%	0.312%
29	11.804	1648	1652	1655	rVB2	32136	32365	1.47%	0.138%
30	11.839	1655	1658	1660	rBV2	80822	83607	3.81%	0.357%
31	11.863	1660	1662	1666	rVB2	40242	33560	1.53%	0.143%
32	12.022	1685	1689	1691	rBV	45683	44189	2.01%	0.188%
33	12.045	1691	1693	1698	rVB	43505	36917	1.68%	0.157%
34	12.280	1729	1733	1736	rBV2	73343	76451	3.48%	0.326%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

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:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.339	1741	1743	1745	rVV2	71449	63261	2.88%	0.270%
36	12.357	1745	1746	1751	rVB3	40437	34377	1.56%	0.147%
37	12.433	1755	1759	1763	rVB	510536	455150	20.72%	1.941%
38	12.492	1763	1769	1773	rBV6	15265	27652	1.26%	0.118%
39	12.663	1789	1798	1801	rBV	495105	518057	23.58%	2.209%
40	12.710	1804	1806	1813	rVB4	25326	33738	1.54%	0.144%
41	12.786	1815	1819	1820	rBV	27915	27183	1.24%	0.116%
42	12.810	1820	1823	1827	rVB	1159202	1043277	47.49%	4.449%
43	12.869	1830	1833	1834	rBV	36410	33550	1.53%	0.143%
44	12.992	1851	1854	1857	rVB	49932	51639	2.35%	0.220%
45	13.057	1862	1865	1868	rVB2	34329	32980	1.50%	0.141%
46	13.092	1868	1871	1874	rBV	62438	66773	3.04%	0.285%
47	13.186	1885	1887	1890	rBV	27480	26303	1.20%	0.112%
48	13.216	1890	1892	1897	rVV	30875	25483	1.16%	0.109%
49	13.374	1914	1919	1921	rBV2	32436	44214	2.01%	0.189%
50	13.492	1936	1939	1945	rVB	53321	57570	2.62%	0.246%
51	13.604	1954	1958	1962	rBV2	47272	73485	3.34%	0.313%
52	13.657	1965	1967	1972	rVV2	31213	50139	2.28%	0.214%
53	13.716	1972	1977	1982	rVB2	123276	170576	7.76%	0.727%
54	13.857	1996	2001	2004	rBV2	751394	870147	39.61%	3.711%
55	13.886	2004	2006	2011	rVB	229651	208169	9.48%	0.888%
56	13.963	2015	2019	2021	rBV2	25923	36451	1.66%	0.155%
57	14.045	2030	2033	2035	rVB2	27718	25722	1.17%	0.110%
58	14.074	2036	2038	2042	rVB2	24175	26305	1.20%	0.112%
59	14.210	2059	2061	2063	rBV2	25879	23661	1.08%	0.101%
60	14.245	2063	2067	2070	rVV	51922	55637	2.53%	0.237%
61	14.280	2070	2073	2075	rVV3	33156	31604	1.44%	0.135%
62	14.621	2126	2131	2140	rBV	597939	705120	32.10%	3.007%
63	14.868	2169	2173	2182	rVB	185468	340342	15.49%	1.451%
64	14.968	2187	2190	2193	rVB	44500	49301	2.24%	0.210%
65	15.151	2217	2221	2227	rVB	107831	131839	6.00%	0.562%
66	15.210	2227	2231	2236	rBV	133670	166549	7.58%	0.710%
67	15.268	2236	2241	2244	rBV	390812	463527	21.10%	1.977%
68	16.621	2466	2471	2477	rVB2	57271	104978	4.78%	0.448%
69	17.027	2535	2540	2548	rVB2	39671	81250	3.70%	0.346%
70	17.409	2598	2605	2614	rVB	82559	208375	9.48%	0.889%

LSC Area Percent Report

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Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
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Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 23449559

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
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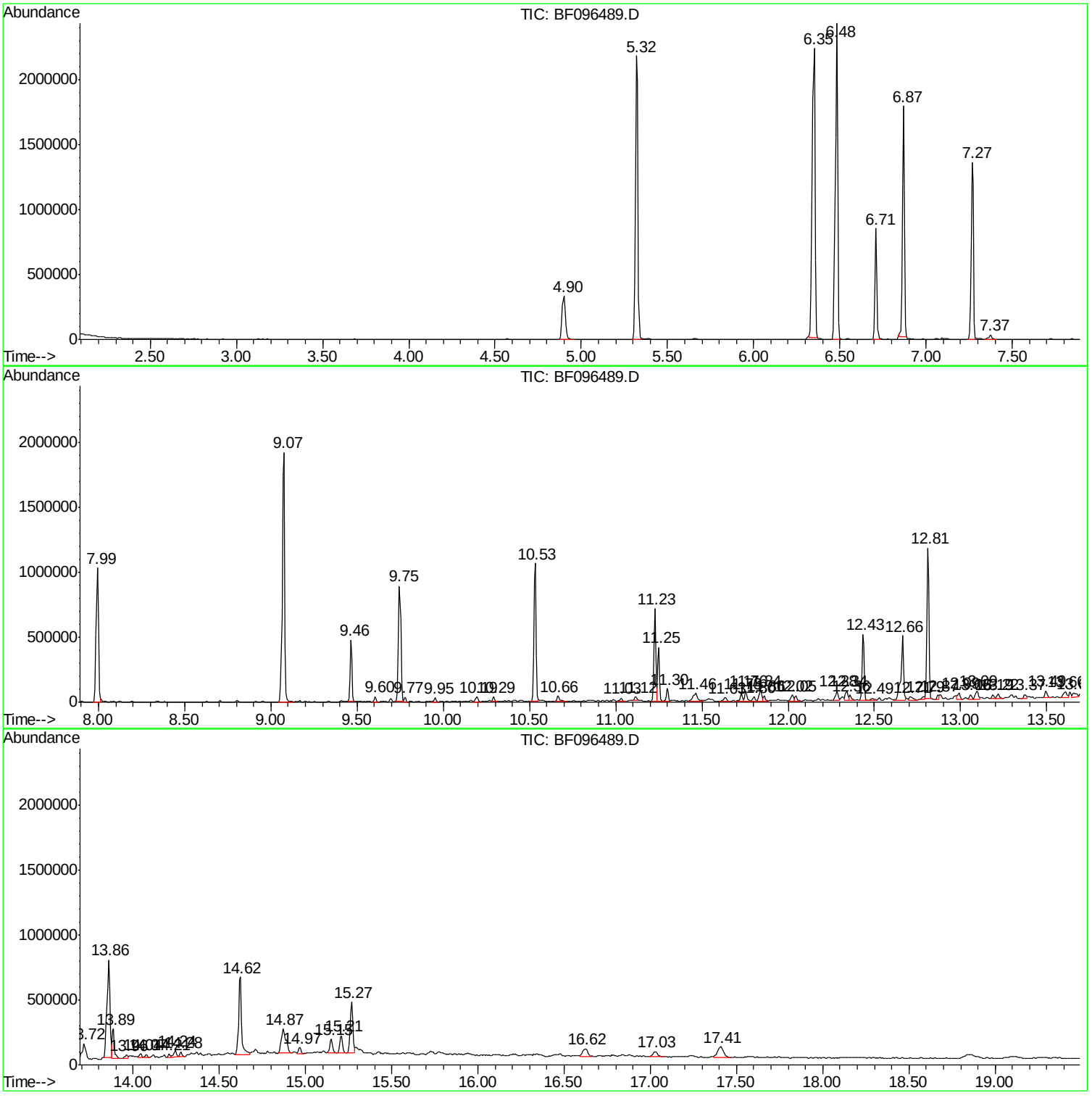
Instrument :
BNA_F
ClientSampleId :
POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

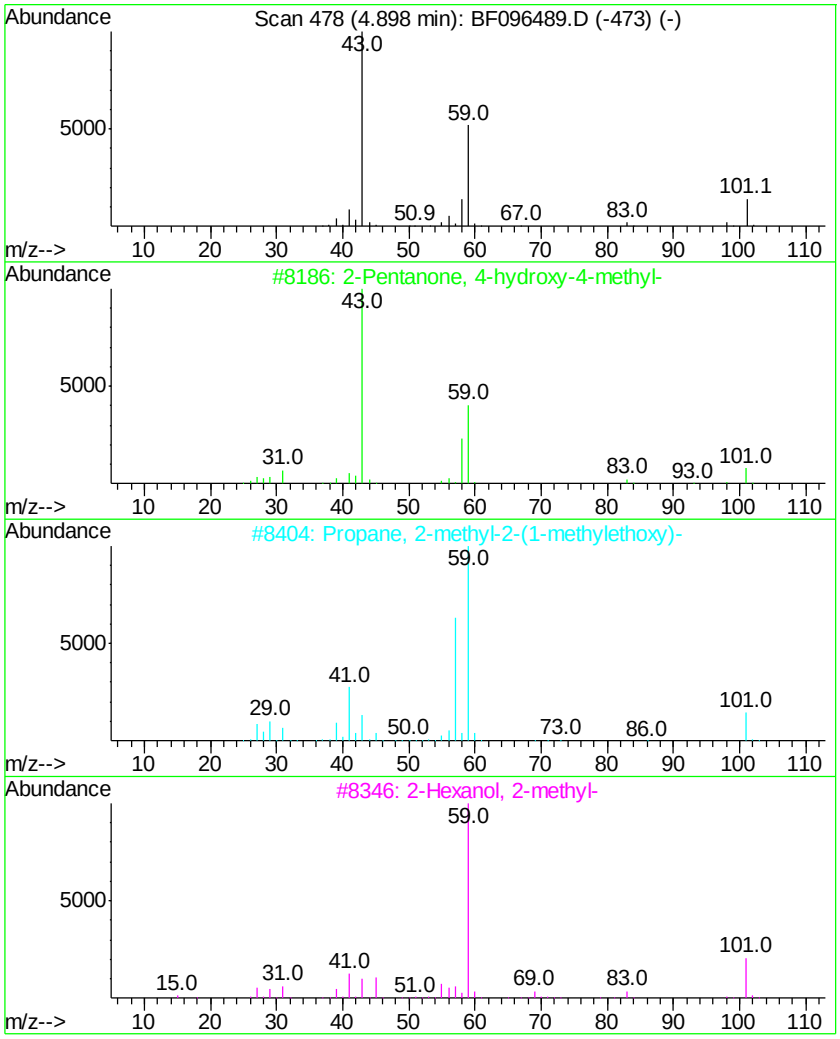
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

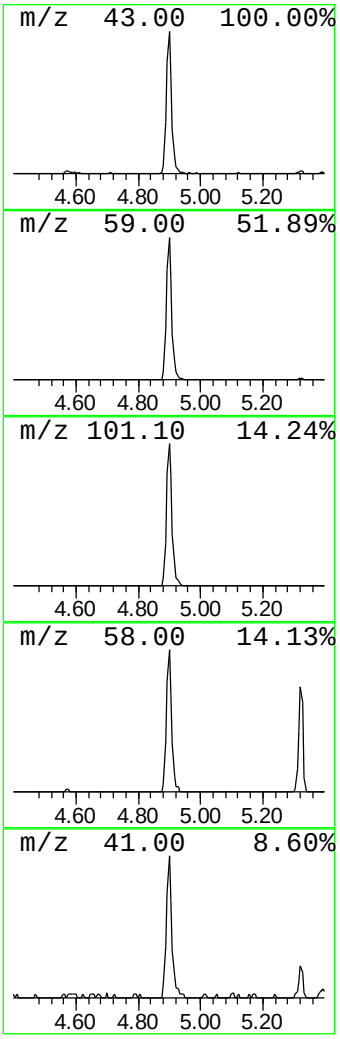
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	11.86 ng	402804	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
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Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

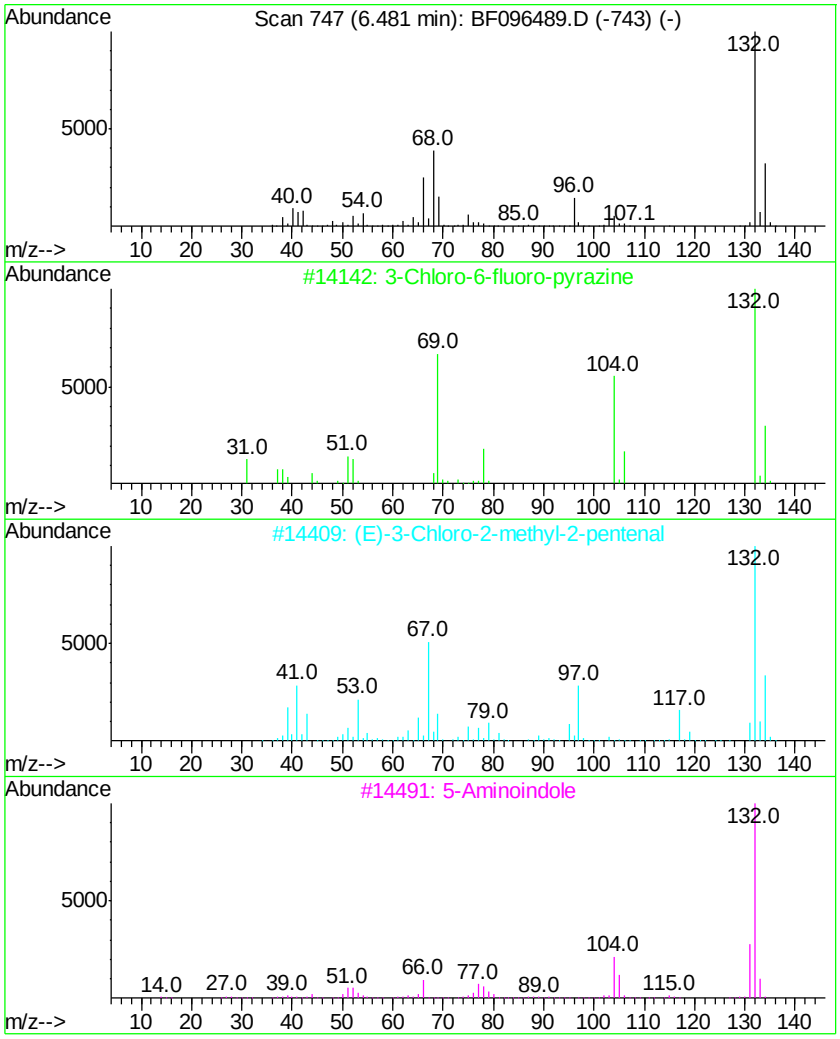
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

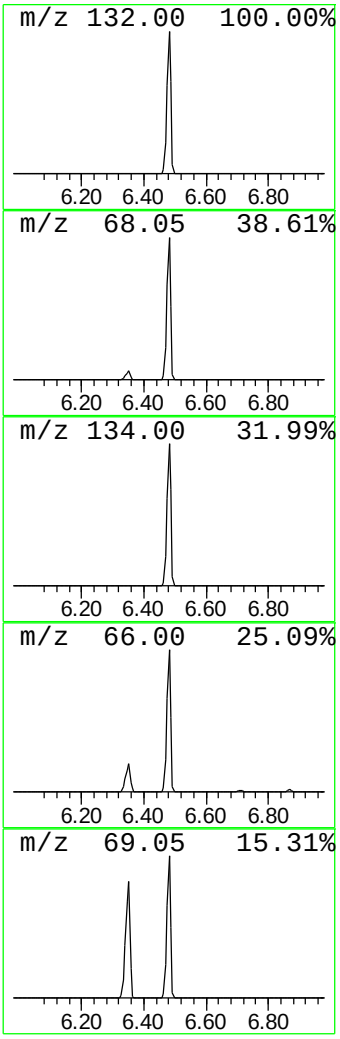
****

Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	63.97 ng	2171990	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

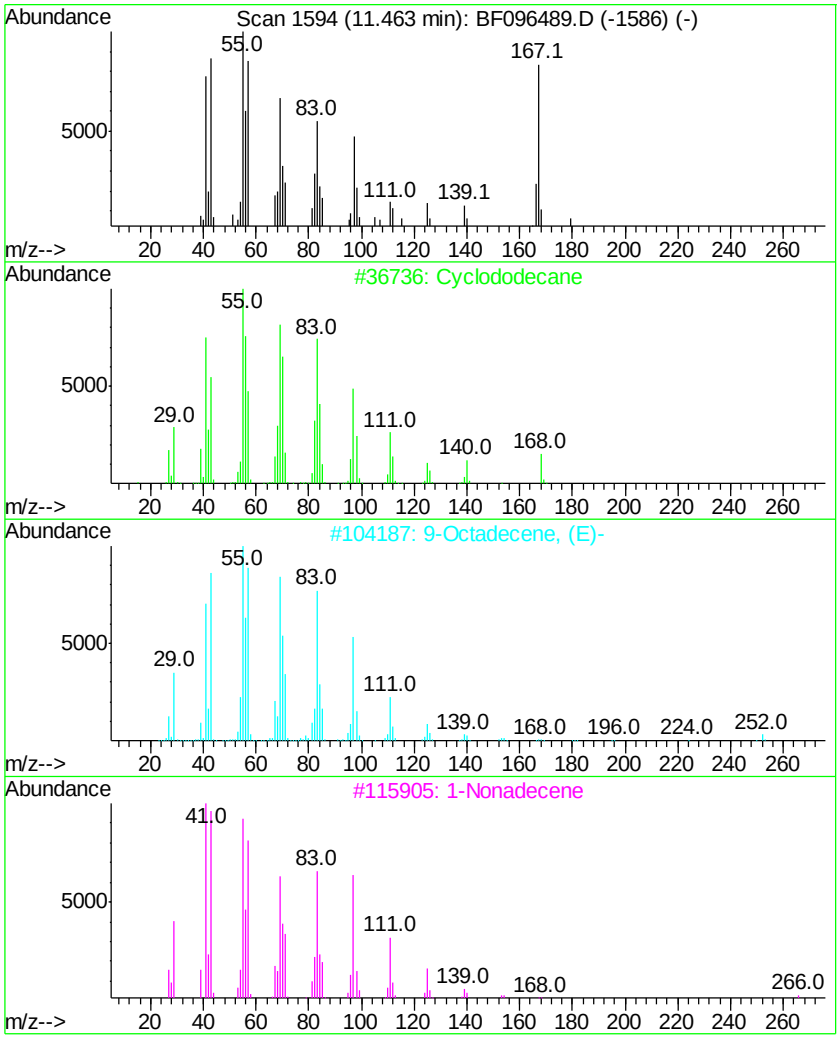
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

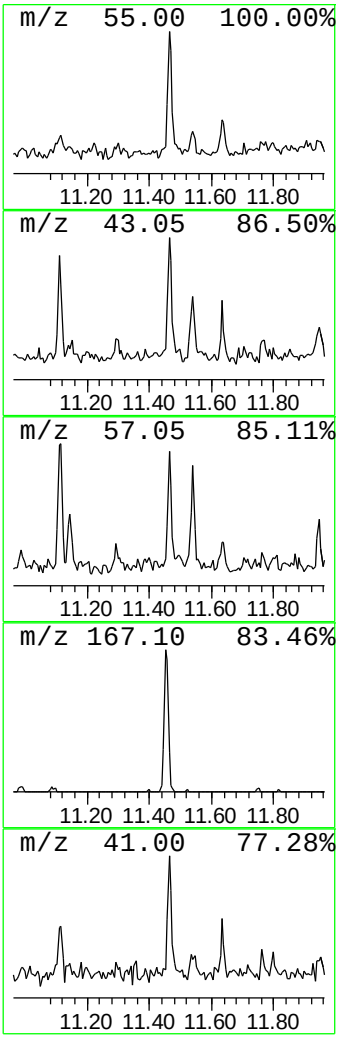
****

Peak Number 4 Cyclododecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	3.13 ng	95268	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecane	168	C12H24	000294-62-2	50
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	43
3	1-Nonadecene	266	C19H38	018435-45-5	43
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	43
5	1-Tridecene	182	C13H26	002437-56-1	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

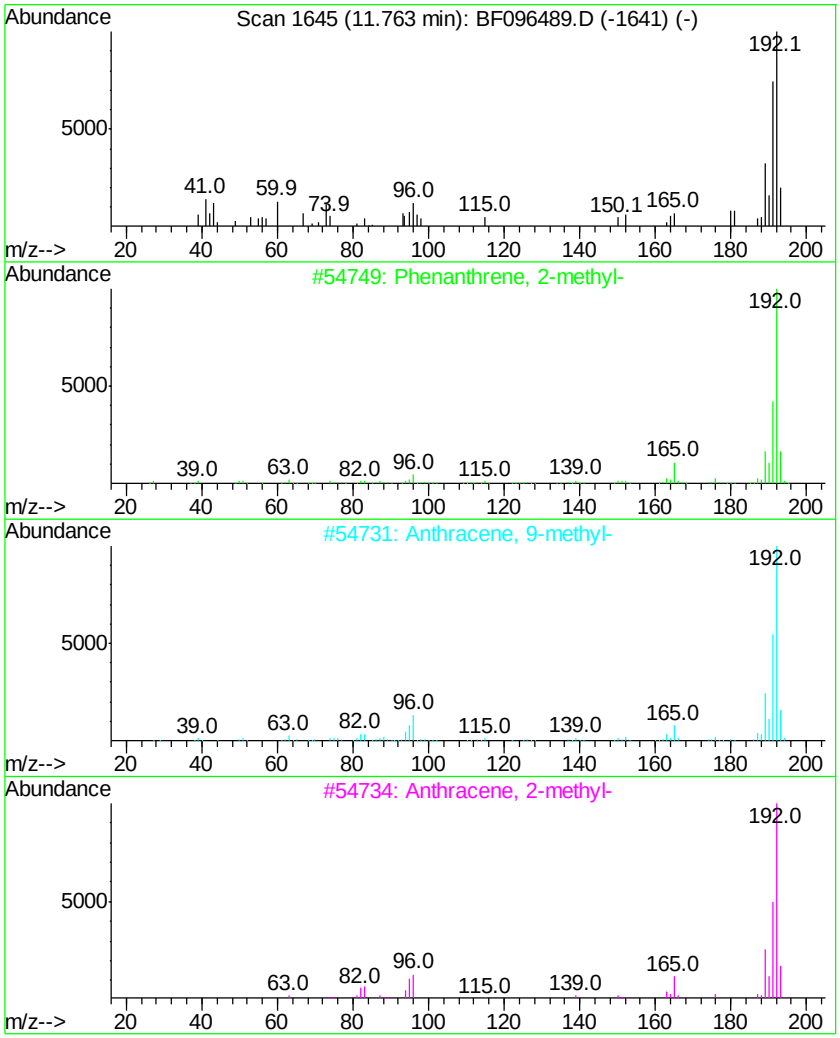
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

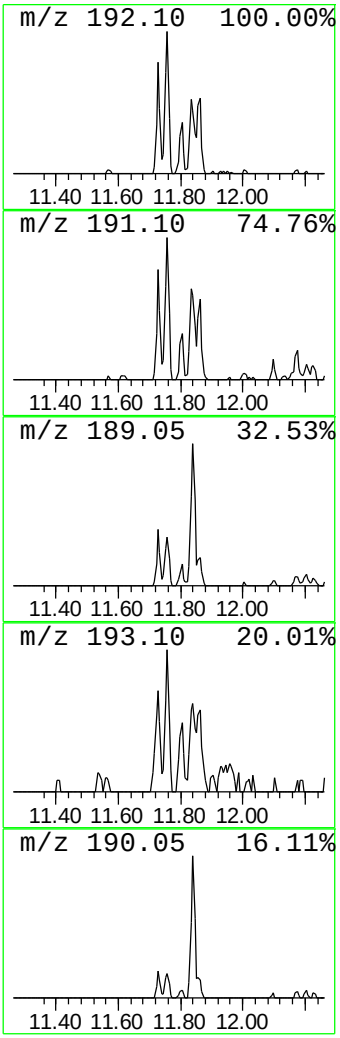
****

Peak Number 5 Phenanthrene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.40 ng	73067	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	91
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	87





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Sample : I3871-08
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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

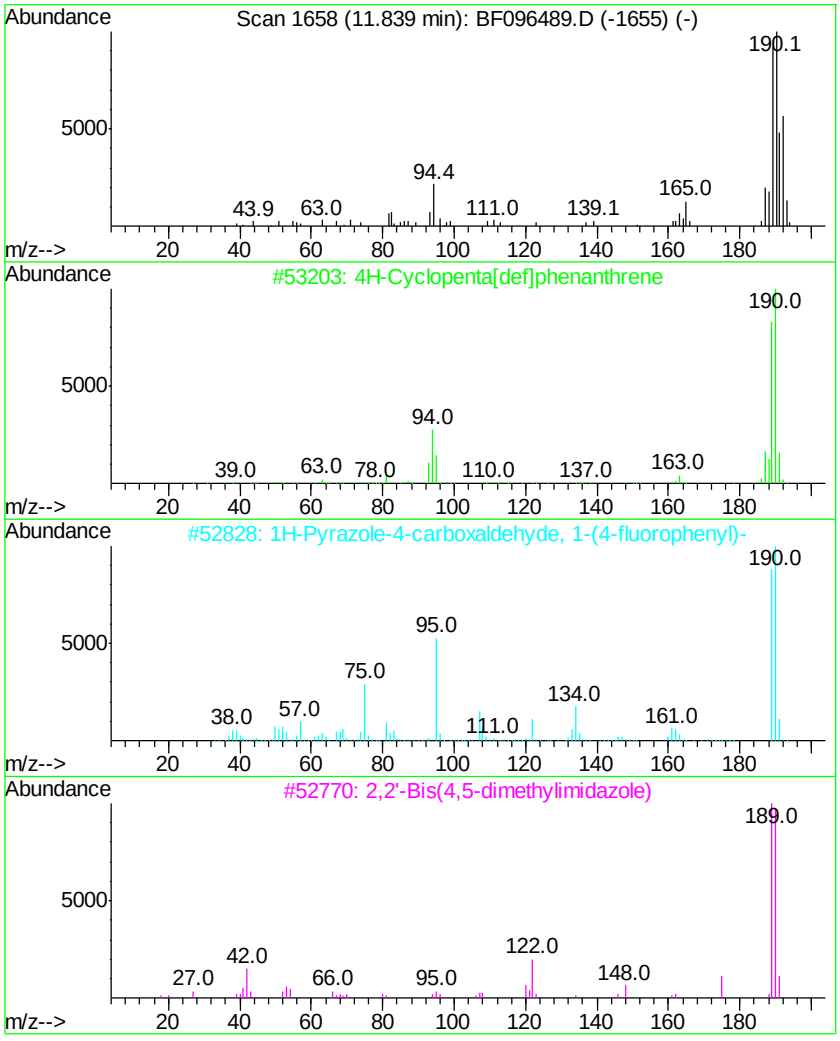
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

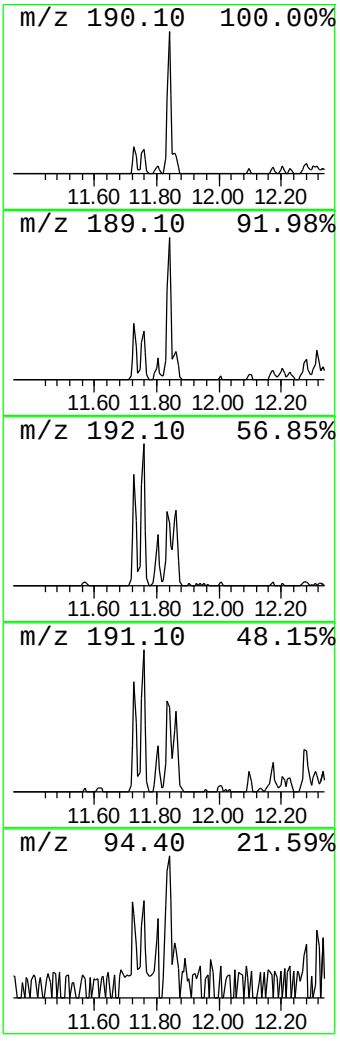
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.74 ng	83607	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	1H-Pyrazole-4-carboxaldehyde, 1-...	190	C10H7FN2O	1000338-05-6	46
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	30
5	2,6-Dichlorobenzaldoxime	189	C7H5Cl2NO	025185-95-9	30





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Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

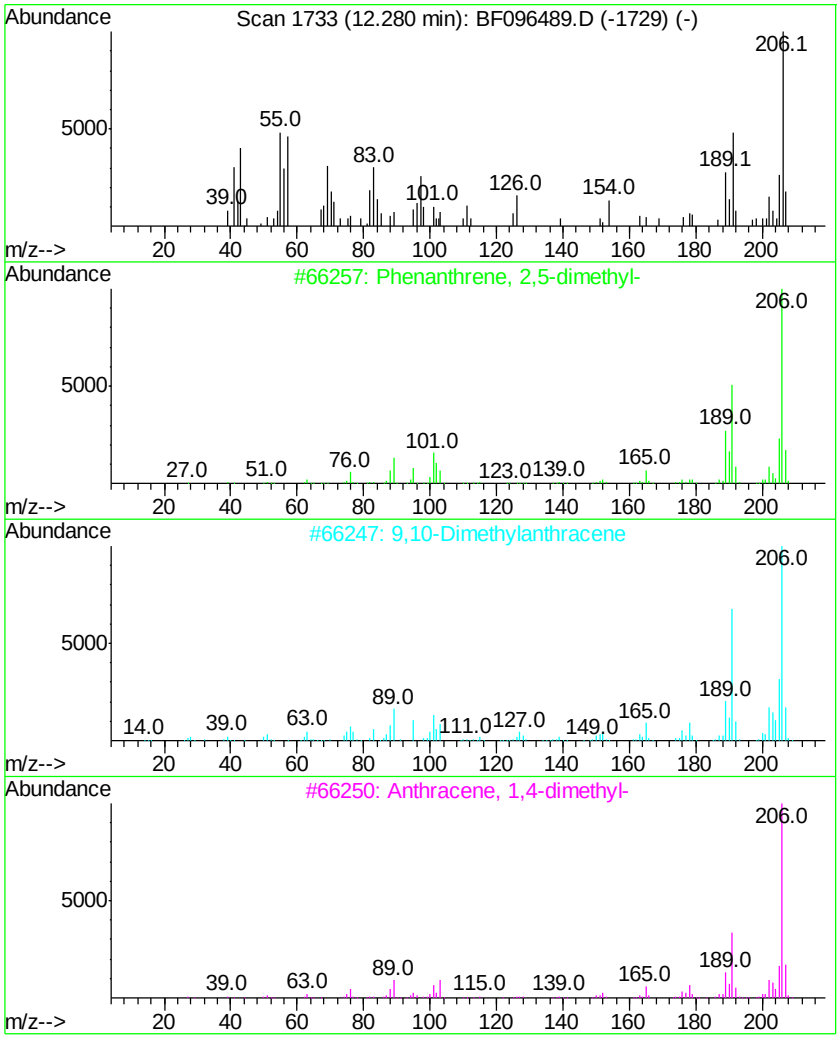
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

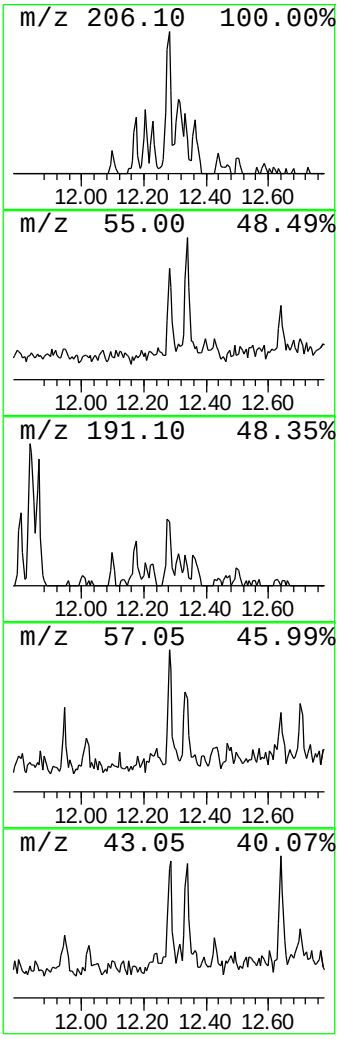
****

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	2.51 ng	76451	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	91
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	90
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	90
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	89
5	di-p-Tolylacetylene	206	C16H14	002789-88-0	89





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Data File : BF096489.D
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Operator : SJ/MA
Sample : I3871-08
Misc :
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Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

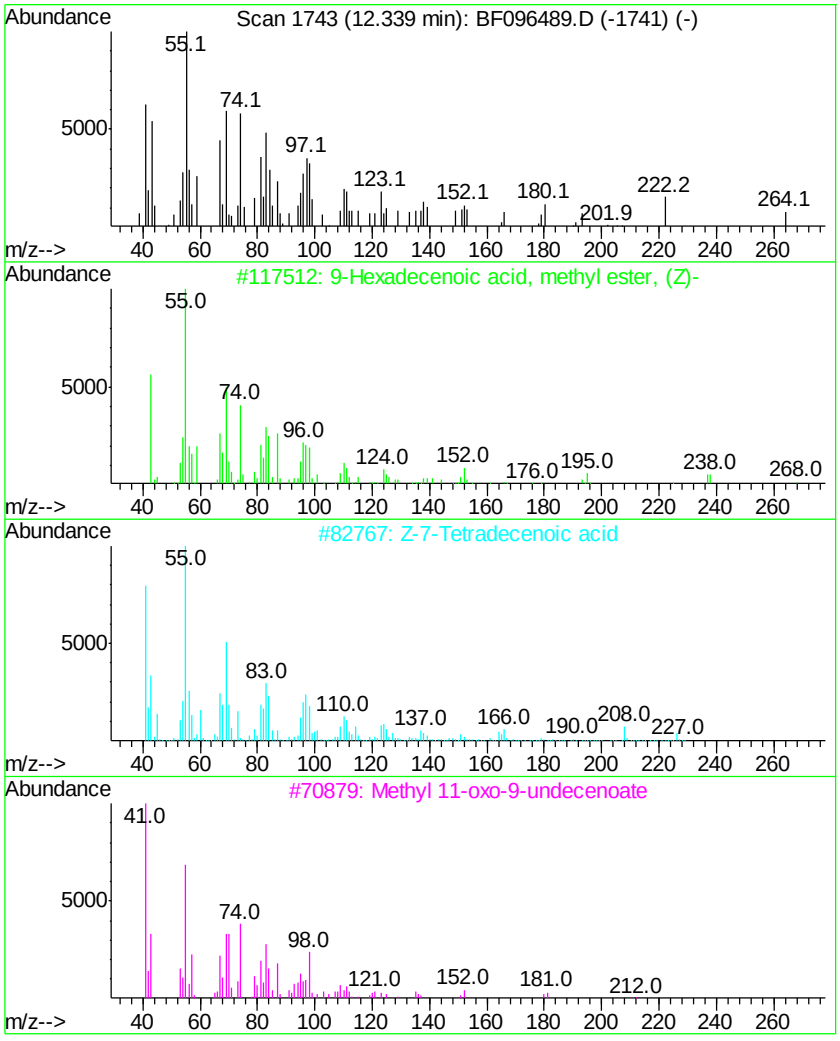
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

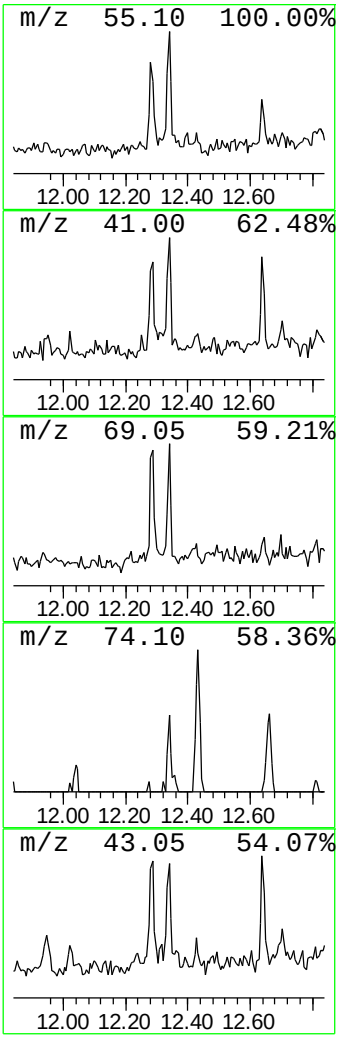
****

Peak Number 8 9-Hexadecenoic acid, methyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	2.08 ng	63261	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	80
2	Z-7-Tetradecenoic acid	226	C14H26O2	1000130-98-4	58
3	Methyl 11-oxo-9-undecenoate	212	C12H20O3	053613-55-1	53
4	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	53
5	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	53





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Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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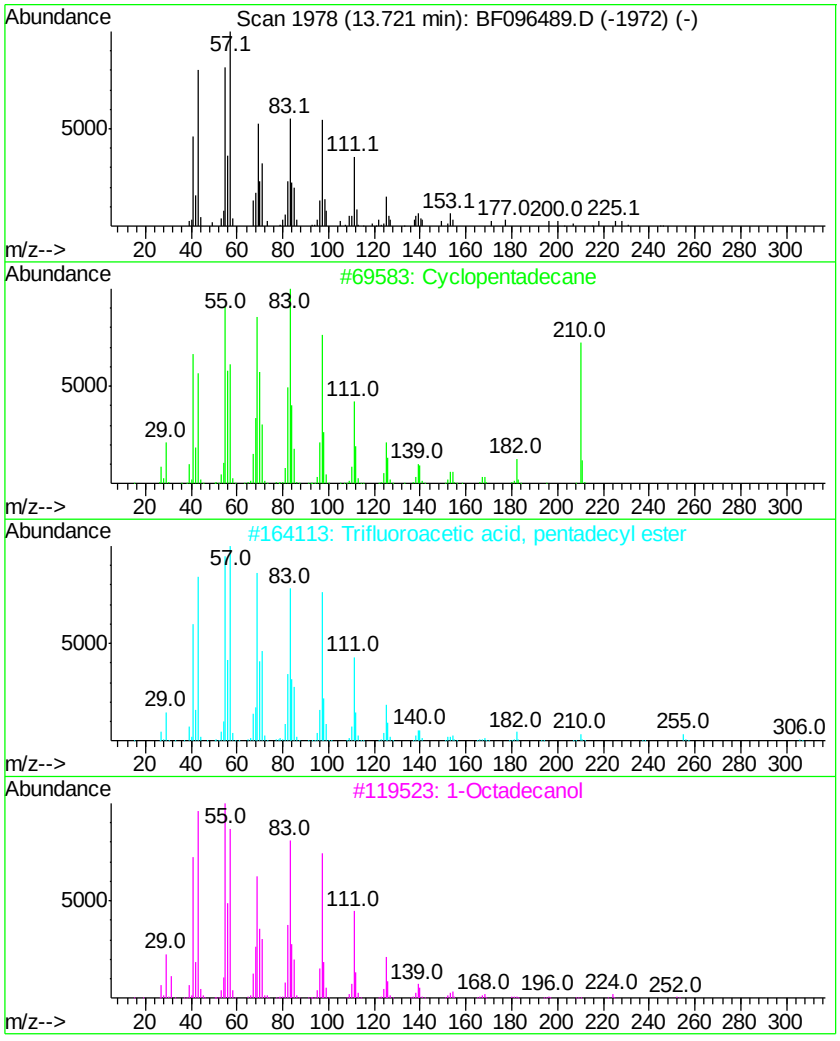
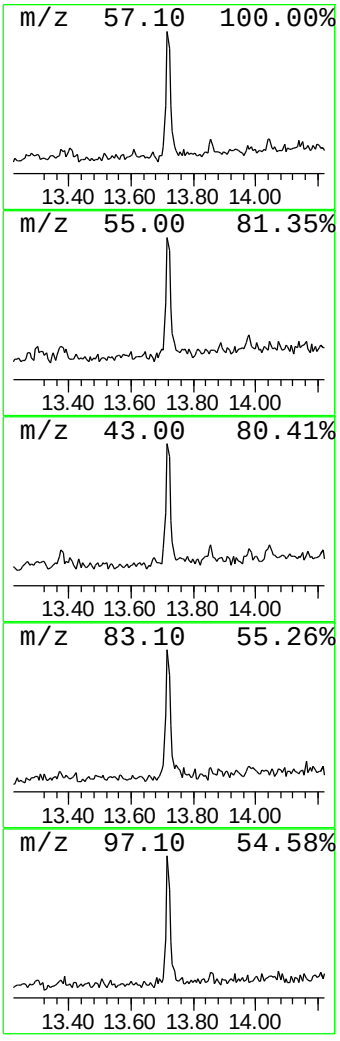
Peak Number 9 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	3.92 ng	170576	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
3	1-Octadecanol	270	C18H38O	000112-92-5	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90





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Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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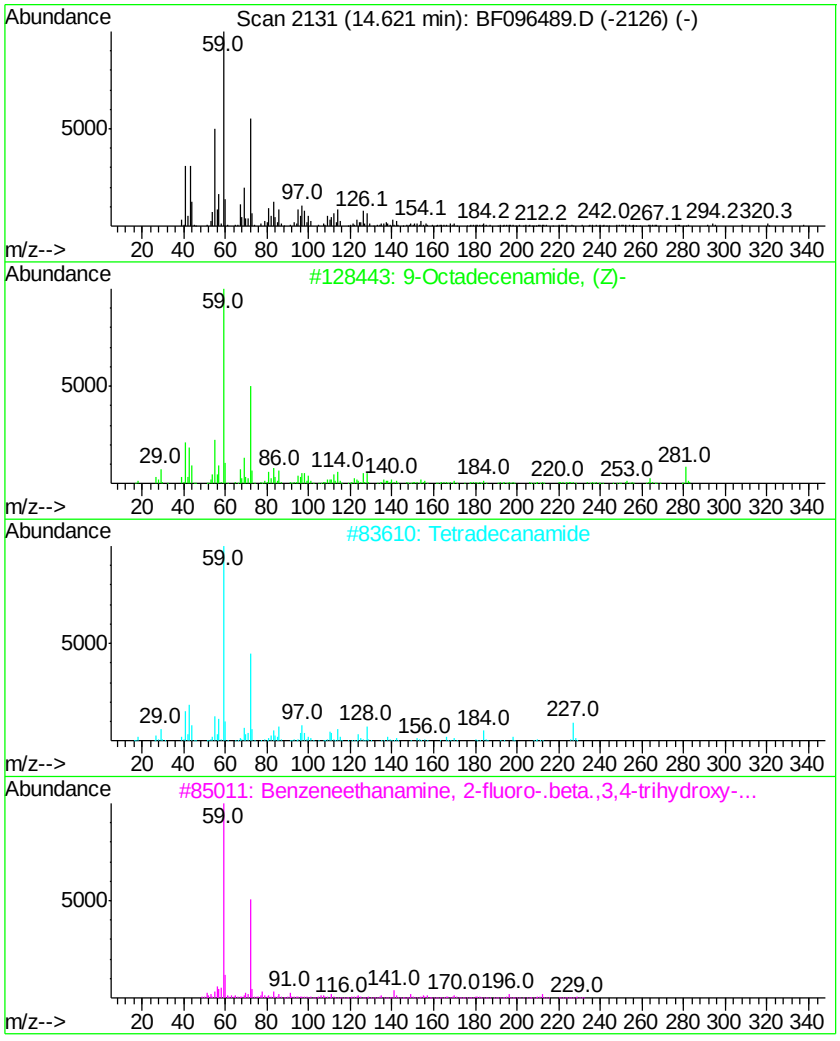
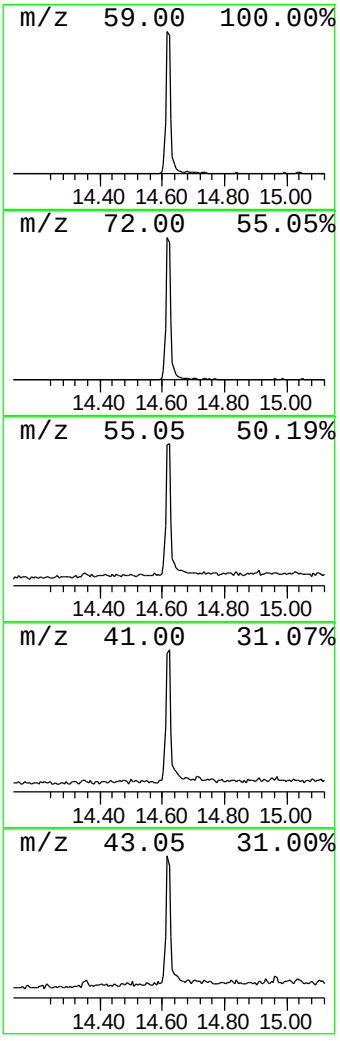
Peak Number 10 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	30.42 ng	705120	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	94
2	Tetradecanamide	227	C14H29NO	000638-58-4	86
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	72
4	Hexadecanamide	255	C16H33NO	000629-54-9	72
5	Octadecanamide	283	C18H37NO	000124-26-5	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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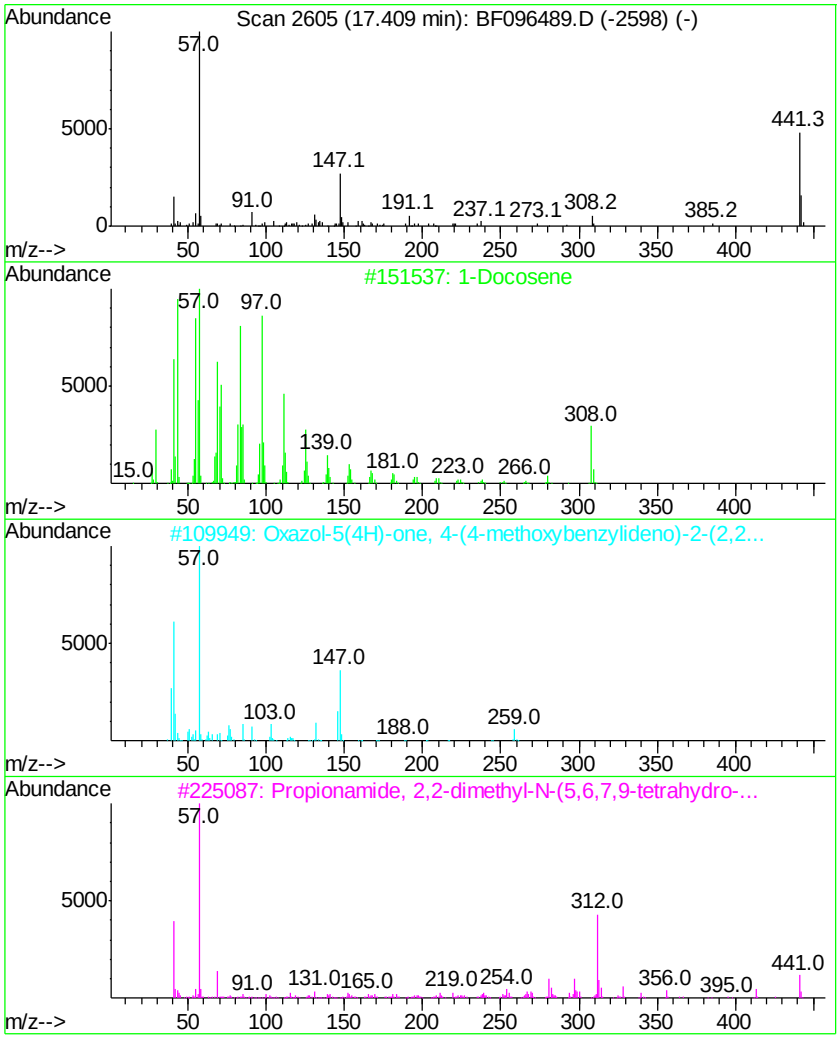
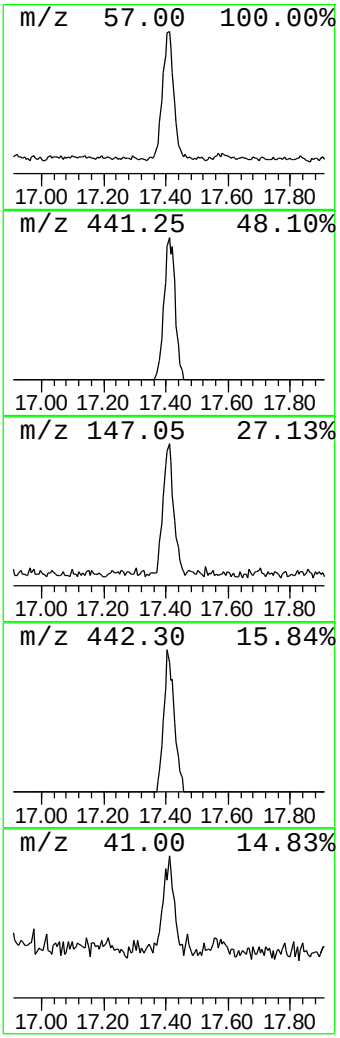
Peak Number 13 unknown17.41 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.41	8.99 ng	208375	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	10
2	Oxazol-5(4H)-one, 4-(4-methoxybe...	259	C15H17NO3	327991-10-6	10
3	Propionamide, 2,2-dimethyl-N-(5,...	441	C25H31NO6	086436-38-6	4
4	1-Azonia-2-borata-3-thiacyclobut...	308	C9H15BF6N2S	134846-06-3	4
5	2-t-Butyl-5-chloromethyl-3-methy...	304	C14H25ClN2O3	1000192-88-5	4





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
Data File : BF096489.D
Acq On : 5 Jul 2017 17:38
Operator : SJ/MA
Sample : I3871-08
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-54-20170622

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	11.9	ng	402804	1	6.71	679084	20.0
unknown6.48	6.48	64.0	ng	2171990	1	6.71	679084	20.0
Cyclododecane	11.46	3.1	ng	95268	4	11.23	609526	20.0
Phenanthrene, 2-m...	11.76	2.4	ng	73067	4	11.23	609526	20.0
4H-Cyclopenta[def...	11.84	2.7	ng	83607	4	11.23	609526	20.0
Phenanthrene, 2,5...	12.28	2.5	ng	76451	4	11.23	609526	20.0
9-Hexadecenoic ac...	12.34	2.1	ng	63261	4	11.23	609526	20.0
Cyclopentadecane	13.72	3.9	ng	170576	5	13.86	870147	20.0
9-Octadecenamide,...	14.62	30.4	ng	705120	6	15.27	463527	20.0
unknown17.41	17.41	9.0	ng	208375	6	15.27	463527	20.0