LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111564.D
Acq On : 18 Dec 2018 2:53
Operator : JU/SJ
Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

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-BF121418.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	3.245	196	197	215	rBV3	72582	157847	4.20%	0.414%
2	4.504	407	411	417	rVB	35154	40208	1.07%	0.105%
3	4.998	491	495	505	rVB	159502	223476	5.95%	0.586%
4	5.422	563	567	582	rBV	3900141	3758796	100.00%	9.858%
5	6.439	735	740	757	rBV	3197092	3758297	99.99%	9.857%
6	6.569	757	762	765	rVV	3640549	3508708	93.35%	9.202%
7	6.622	768	771	776	rVB3	33178	44080	1.17%	0.116%
8	6.786	796	799	803	rBV	1009411	813499	21.64%	2.134%
9	6.945	822	826	829	rBV	3024404	2639724	70.23%	6.923%
10	7.351	889	895	898	rBV	2344044	2182051	58.05%	5.723%
11	8.069	1013	1017	1037	rVB	1184371	1044716	27.79%	2.740%
12	9.145	1195	1200	1203	rBV	3889182	3526360	93.82%	9.249%
13	9.539	1263	1267	1278	rVB	437698	376186	10.01%	0.987%
14	9.821	1311	1315	1319	rBV	1164980	1004102	26.71%	2.633%
15	10.610	1445	1449	1453	rBV	2329773	2347934	62.47%	6.158%
16	10.733	1467	1470	1477	rVB3	35128	57848	1.54%	0.152%
17	11.168	1539	1544	1548	rBV4	95064	115460	3.07%	0.303%
18	11.310	1564	1568	1570	rBV	1182067	1165666	31.01%	3.057%
19	11.327	1570	1571	1575	rVV	299983	232842	6.19%	0.611%
20	11.380	1577	1580	1584	rVB	74090	73820	1.96%	0.194%
21	11.768	1643	1646	1650	rBV3	47719	76079	2.02%	0.200%
22	11.839	1655	1658	1662	rVV	416236	395192	10.51%	1.036%
23	11.868	1662	1663	1668	rVB2	54495	52722	1.40%	0.138%
24	11.921	1668	1672	1674	rBV	78539	74850	1.99%	0.196%
25	12.357	1743	1746	1750	rBV2	55209	59023	1.57%	0.155%
26	12.398	1750	1753	1758	rVV3	72562	96123	2.56%	0.252%
27	12.445	1758	1761	1765	rVB3	31584	38725	1.03%	0.102%
28	12.515	1770	1773	1777	rBV	507116	492863	13.11%	1.293%
29	12.621	1788	1791	1797	rBV4	79885	130457	3.47%	0.342%
30	12.745	1807	1812	1815	rBV	523266	489883	13.03%	1.285%
31	12.774	1815	1817	1819	rVV2	62780	51983	1.38%	0.136%
32	12.792	1819	1820	1826	rVB3	49399	48405	1.29%	0.127%
33	12.892	1833	1837	1845	rVB	3447857	3203667	85.23%	8.402%
34	13.074	1865	1868	1871	rVB	82290	79974	2.13%	0.210%

LSC Area Percent Report

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Operator : JU/SJ
Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

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-BF121418.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.127	1875	1877	1882	rVB2	67146	93106	2.48%	0.244%
36	13.180	1883	1886	1889	rVB2	44928	45510	1.21%	0.119%
37	13.468	1933	1935	1939	rBV	65459	56758	1.51%	0.149%
38	13.580	1952	1954	1959	rVB	55121	60748	1.62%	0.159%
39	13.745	1980	1982	1986	rBV2	32880	38654	1.03%	0.101%
40	13.798	1987	1991	1998	rVB3	274158	377245	10.04%	0.989%
41	13.945	2011	2016	2019	rBV2	1353278	1503205	39.99%	3.942%
42	13.968	2019	2020	2026	rVB	289794	208337	5.54%	0.546%
43	14.051	2032	2034	2037	rVB2	60137	49901	1.33%	0.131%
44	14.115	2042	2045	2050	rVV2	168362	158852	4.23%	0.417%
45	14.421	2094	2097	2101	rBV	266737	259090	6.89%	0.680%
46	14.721	2145	2148	2151	rBV	228125	199362	5.30%	0.523%
47	14.792	2158	2160	2164	rVB	128123	119439	3.18%	0.313%
48	14.968	2187	2190	2199	rVB	247602	457228	12.16%	1.199%
49	15.051	2200	2204	2206	rBV	255530	267852	7.13%	0.703%
50	15.262	2237	2240	2246	rVB	162585	211684	5.63%	0.555%
51	15.321	2247	2250	2254	rVV	200155	239789	6.38%	0.629%
52	15.386	2257	2261	2264	rVV	741153	929596	24.73%	2.438%
53	15.415	2264	2266	2271	rVB	258745	300332	7.99%	0.788%
54	15.839	2334	2338	2342	rVB	145019	190129	5.06%	0.499%

Sum of corrected areas: 38128383

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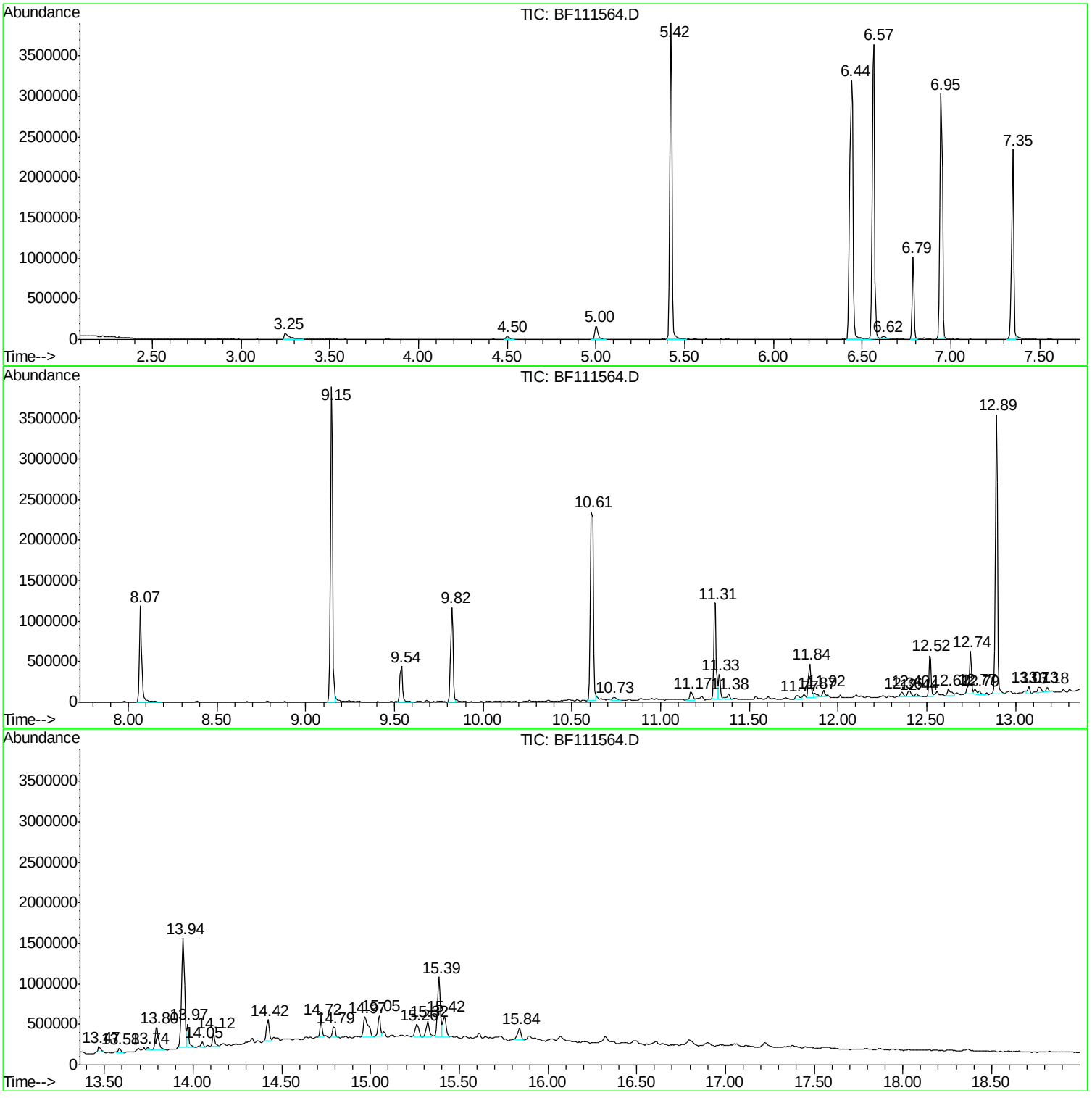
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
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TIC Library : C:\DATABASE\NIST11.L
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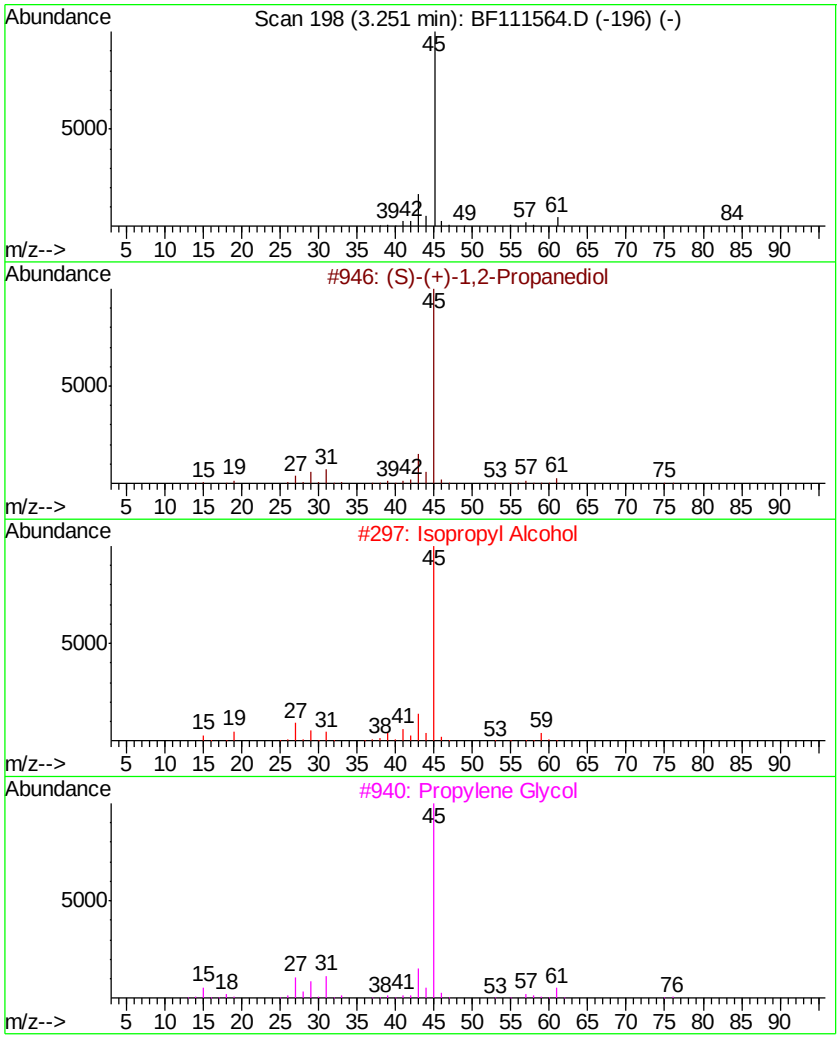
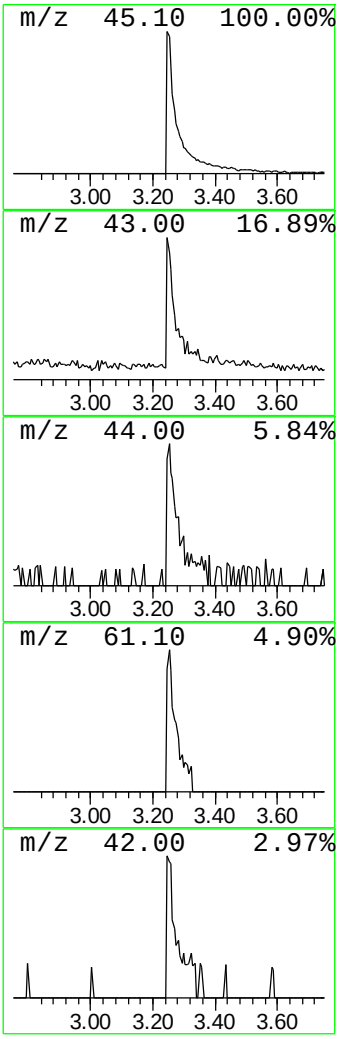
Peak Number 1 unknown3.25 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.25	3.88 ng	157847	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	Muramic acid	251	C9H17NO7	001114-41-6	9





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Operator : JU/SJ
Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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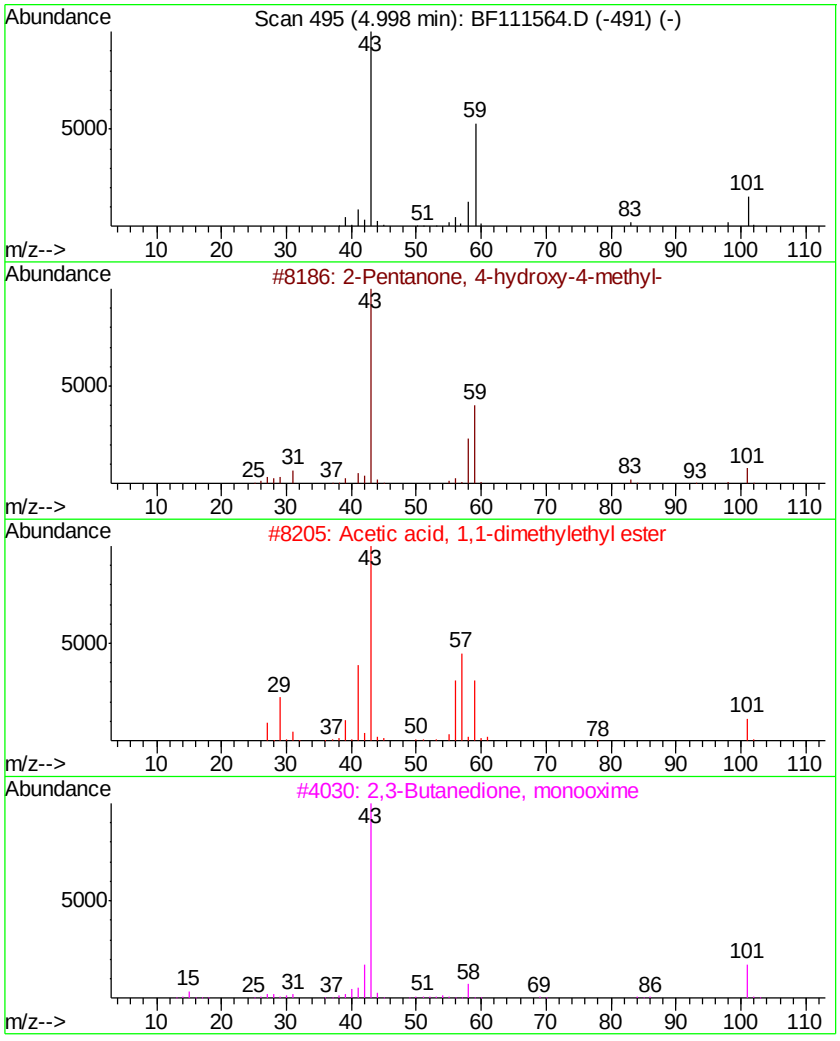
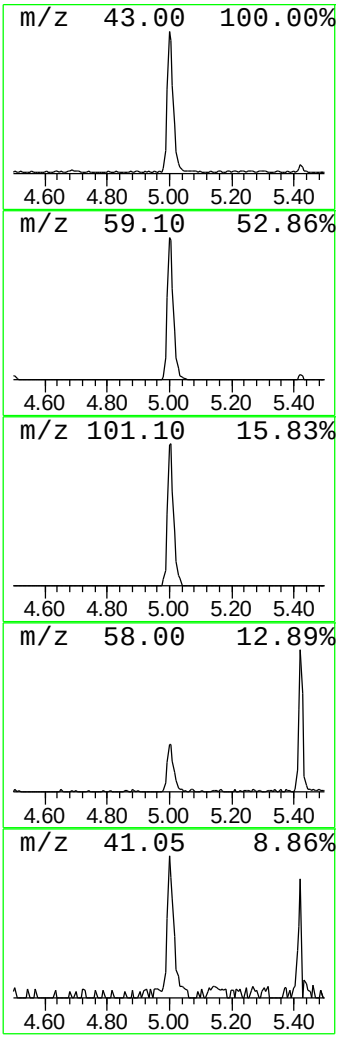
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	5.49 ng	223476	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9





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Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

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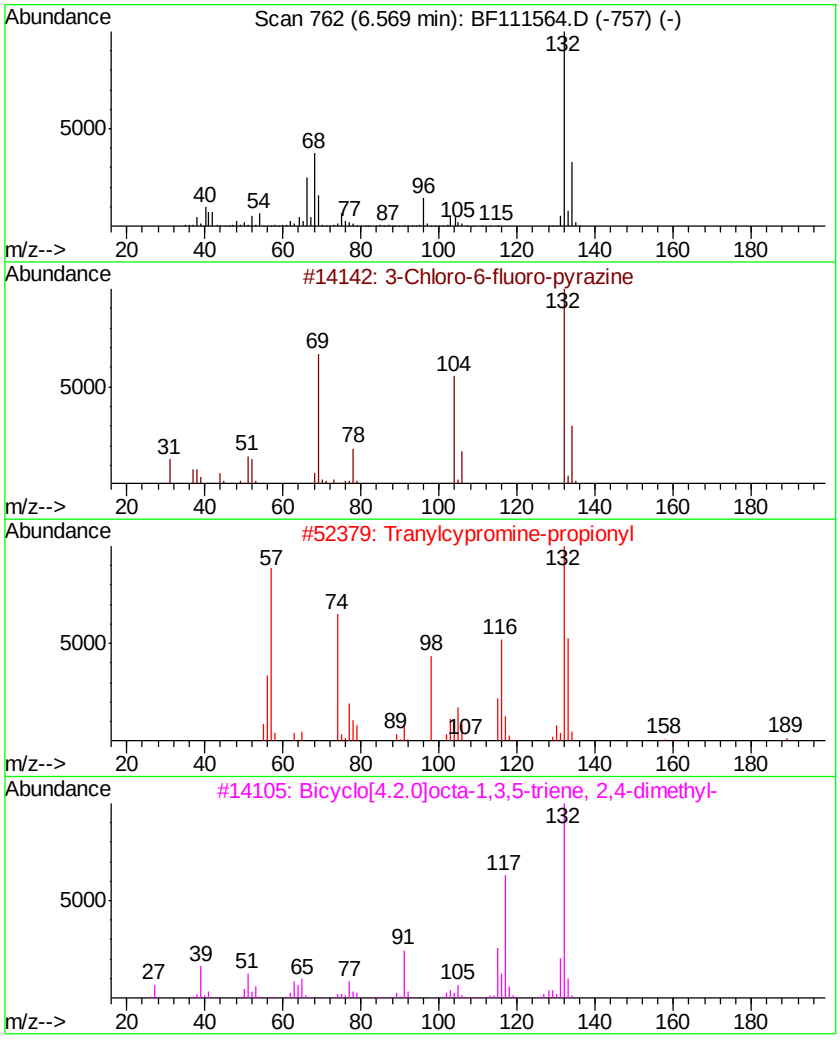
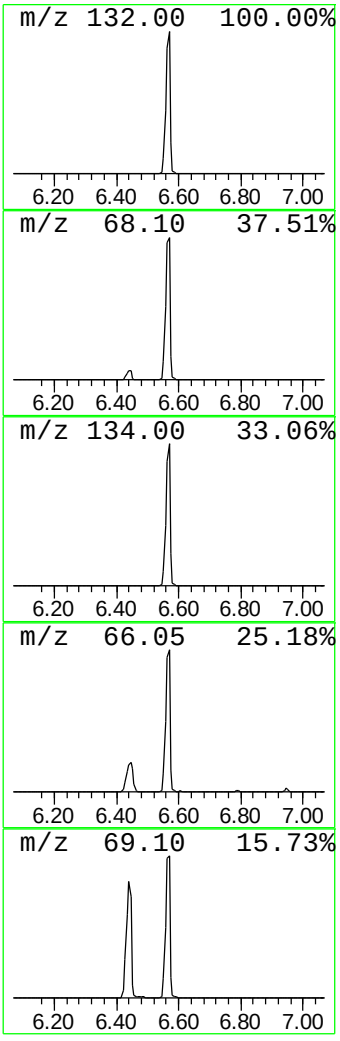
****

Peak Number 3 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	86.26 ng	3508710	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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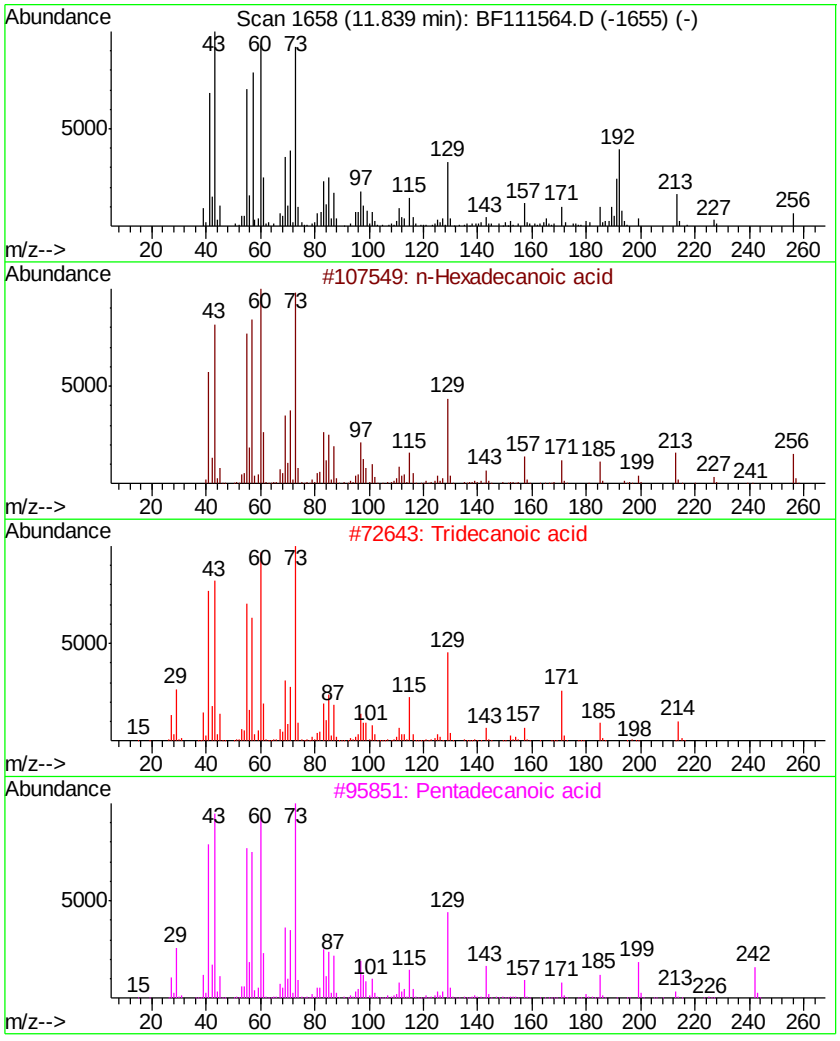
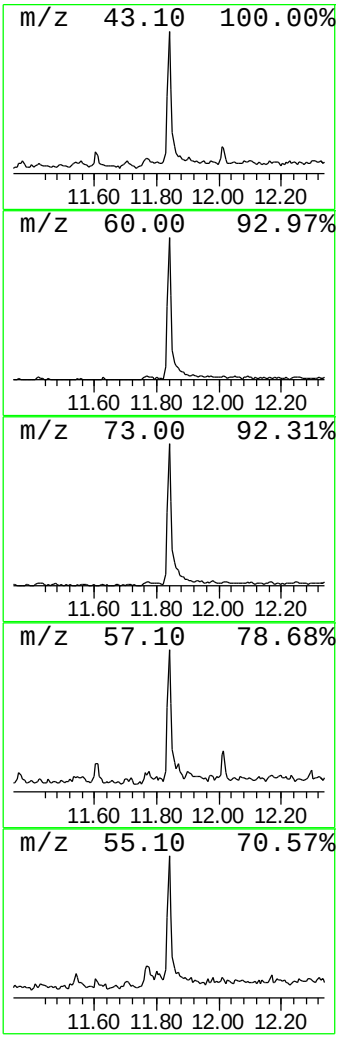
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	6.78 ng	395192	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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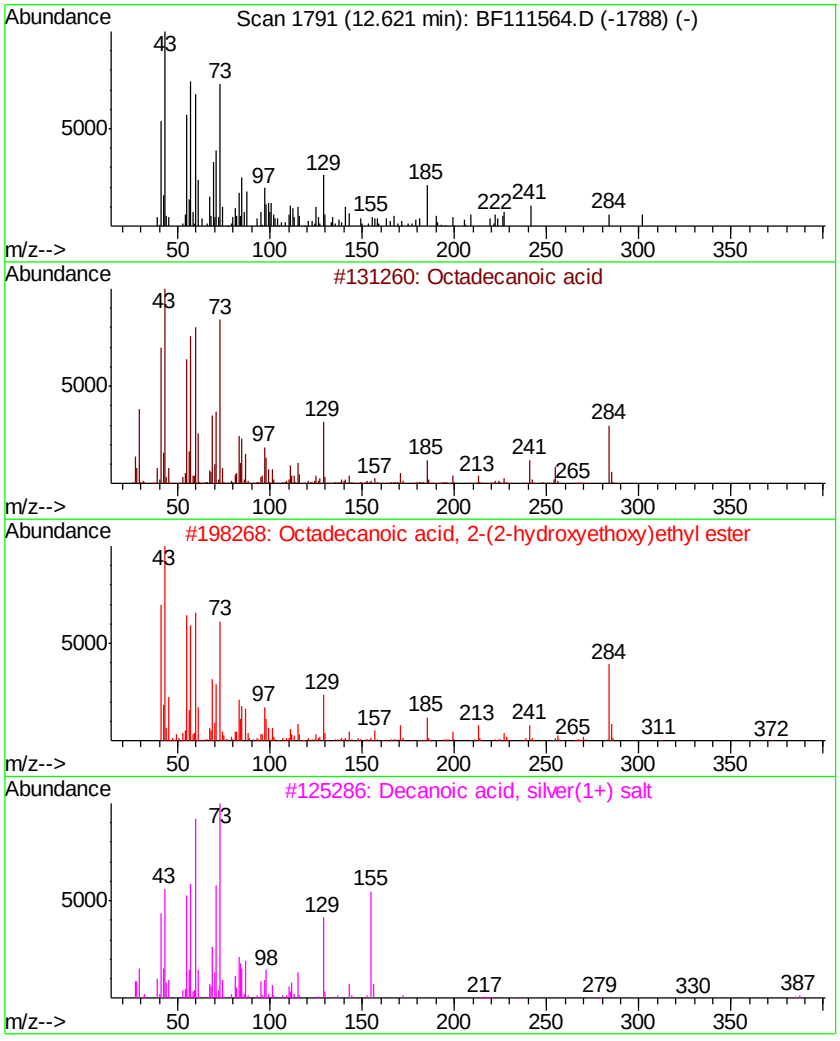
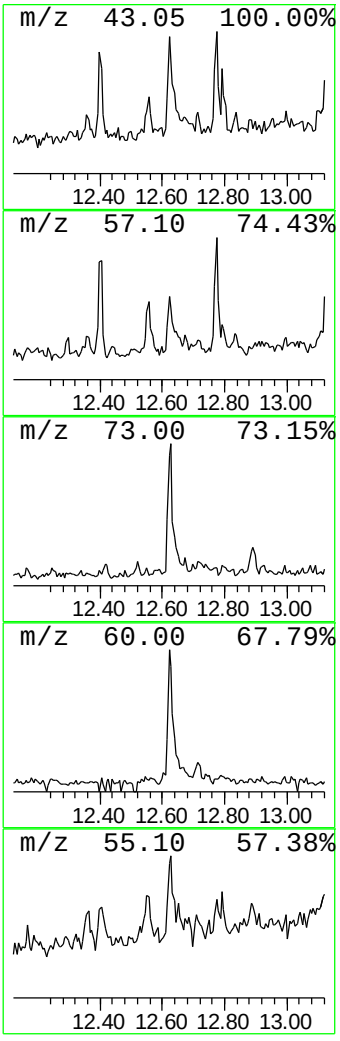
Peak Number 6 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	2.24 ng	130457	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58
4	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	47
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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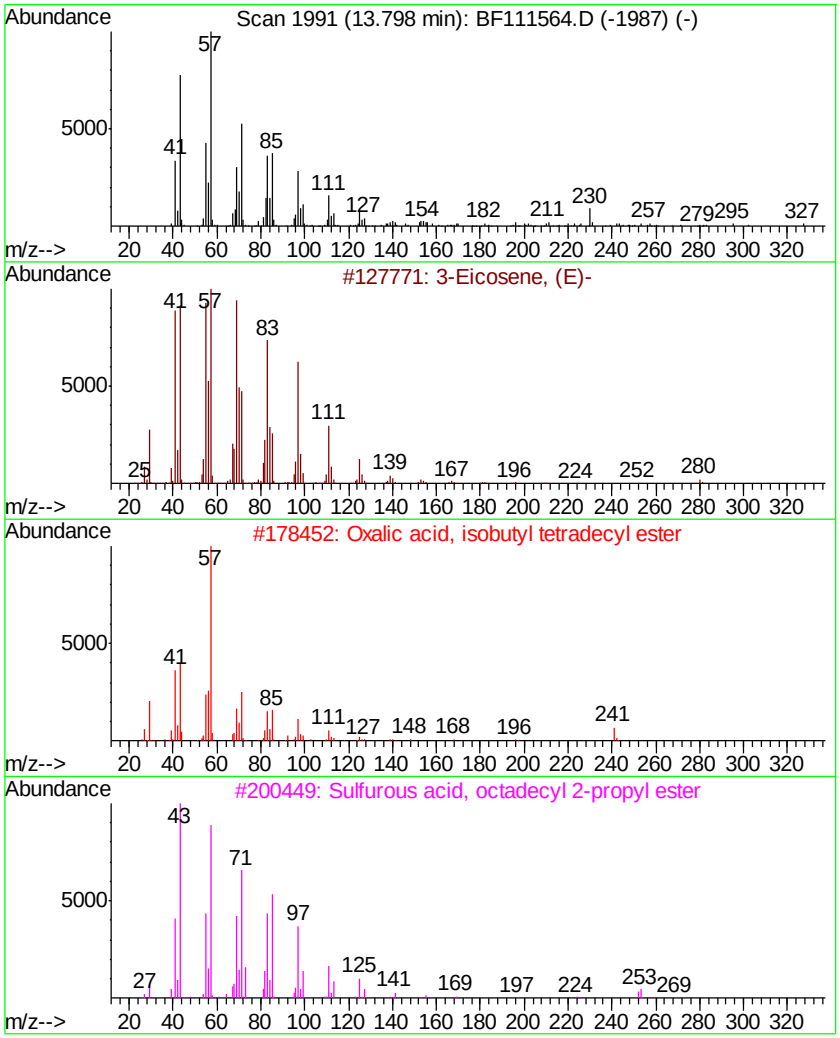
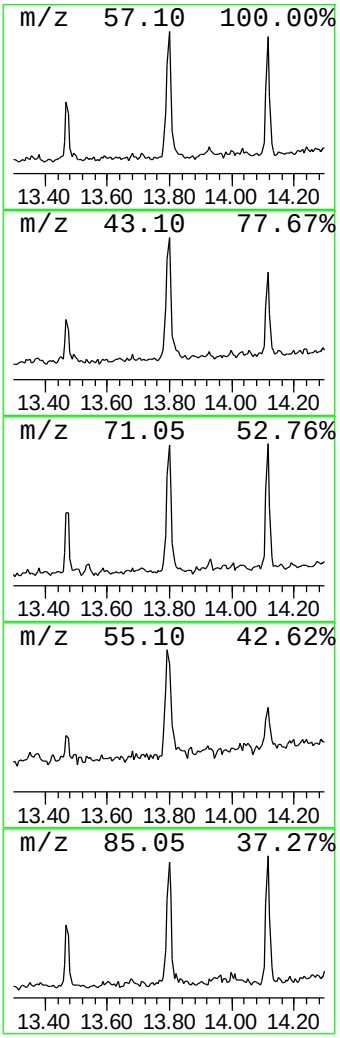
Peak Number 7 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	5.02 ng	377245	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	83





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Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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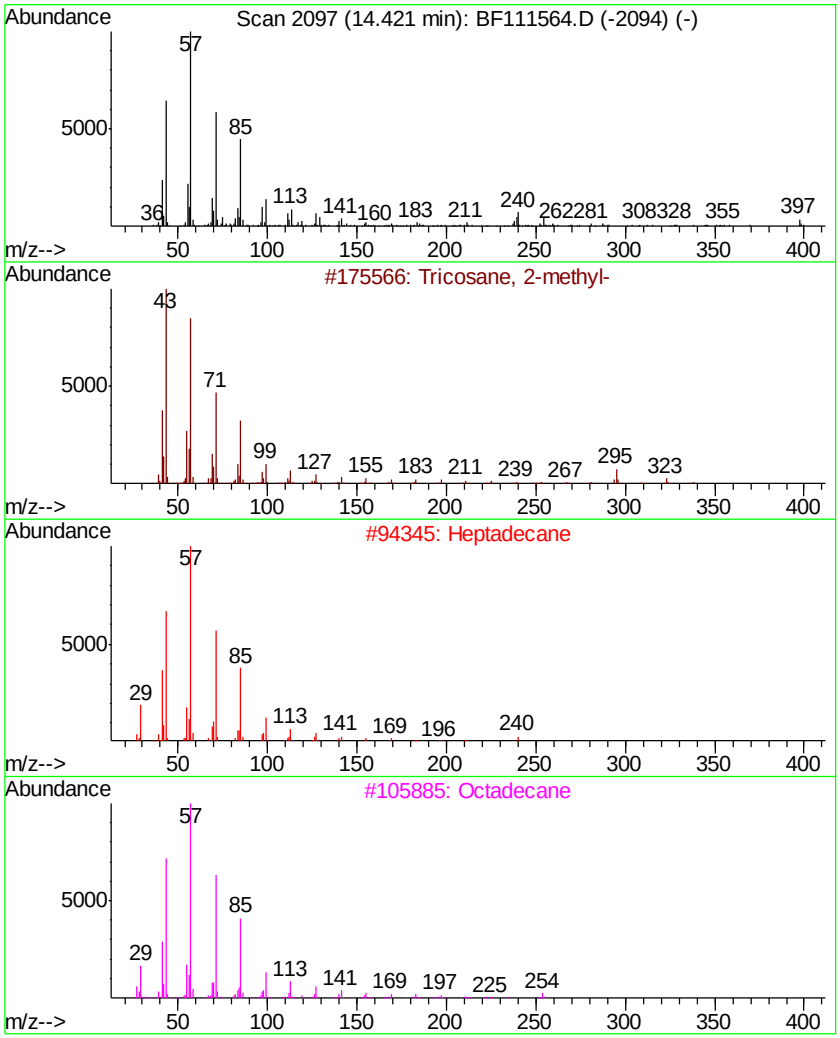
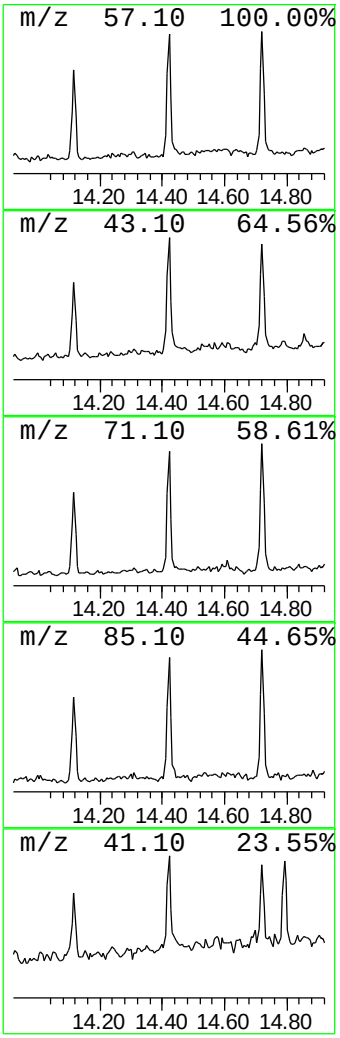
Peak Number 9 Tricosane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	3.45 ng	259090	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosane, 2-methyl-	338	C24H50	001928-30-9	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Octadecane, 2-methyl-	268	C19H40	001560-88-9	87
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	83





Library Search Compound Report

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.M
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TIC Library : C:\DATABASE\NIST11.L
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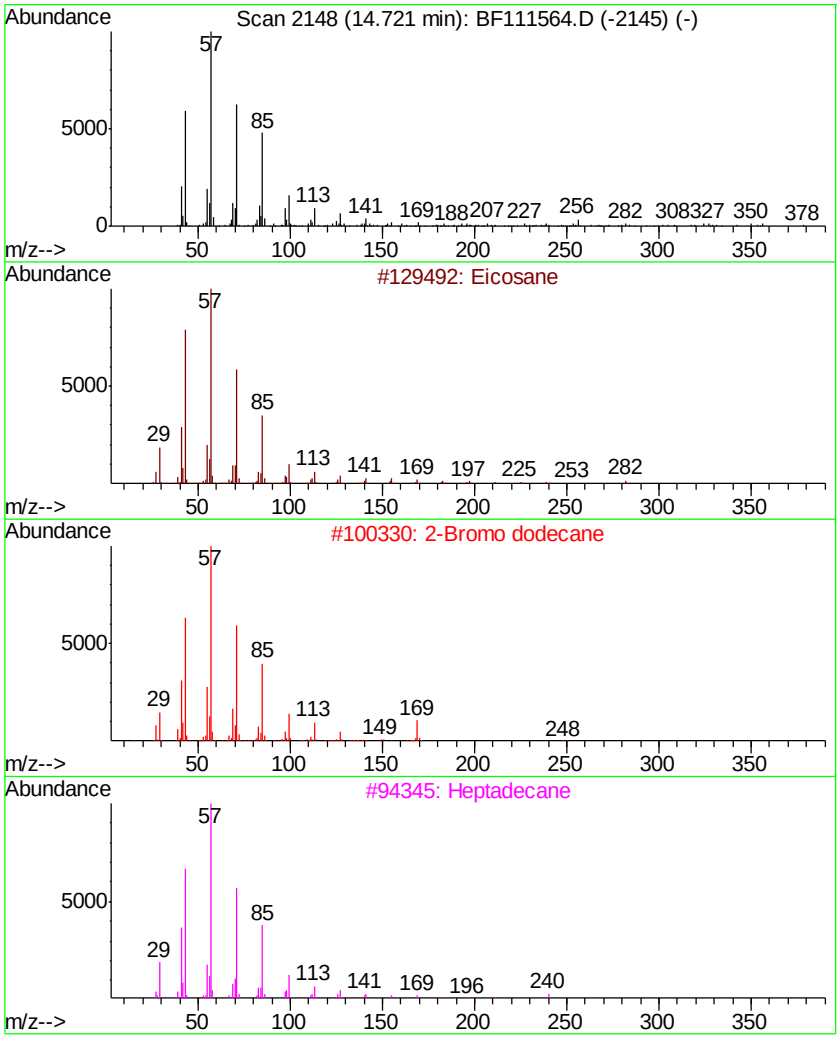
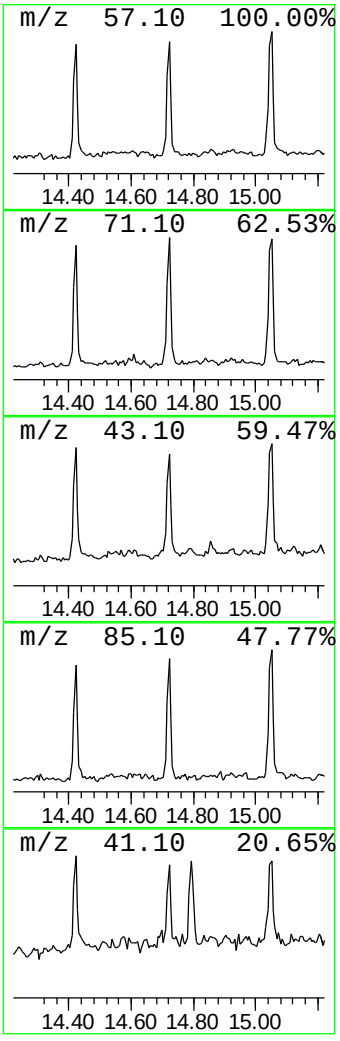
Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	4.29 ng	199362	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3	Heptadecane	240	C17H36	000629-78-7	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Hexadecane	226	C16H34	000544-76-3	86





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Data File : BF111564.D
Acq On : 18 Dec 2018 2:53
Operator : JU/SJ
Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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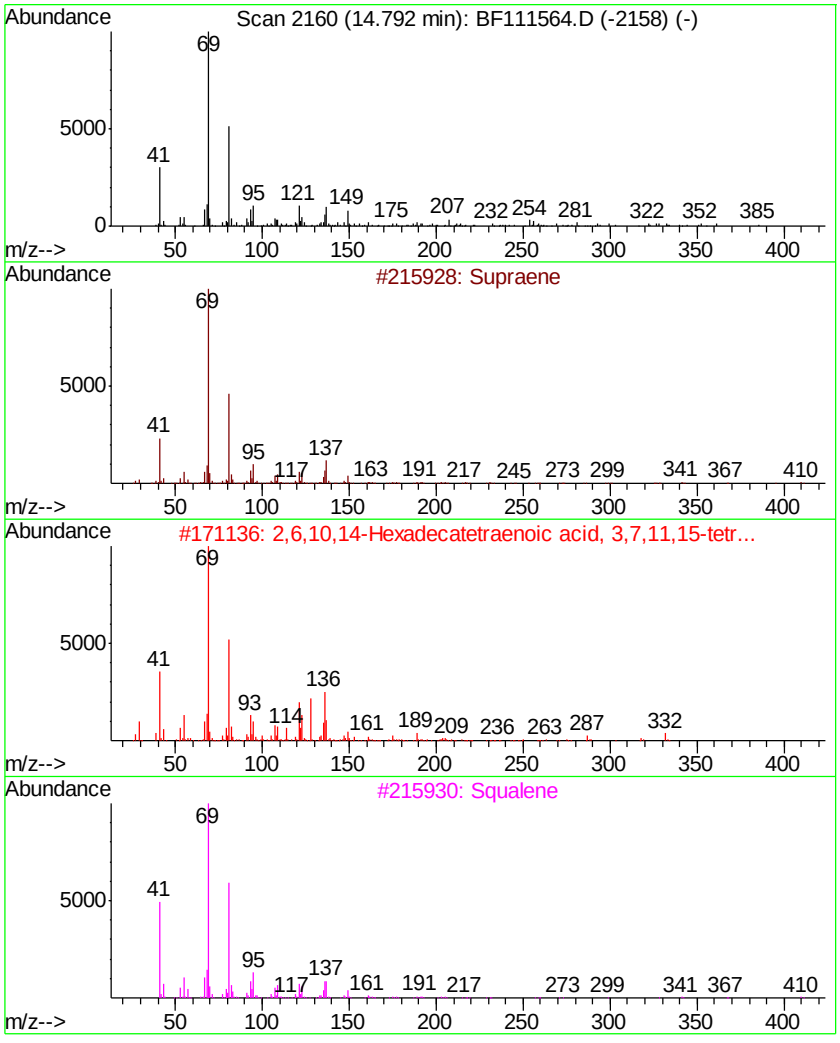
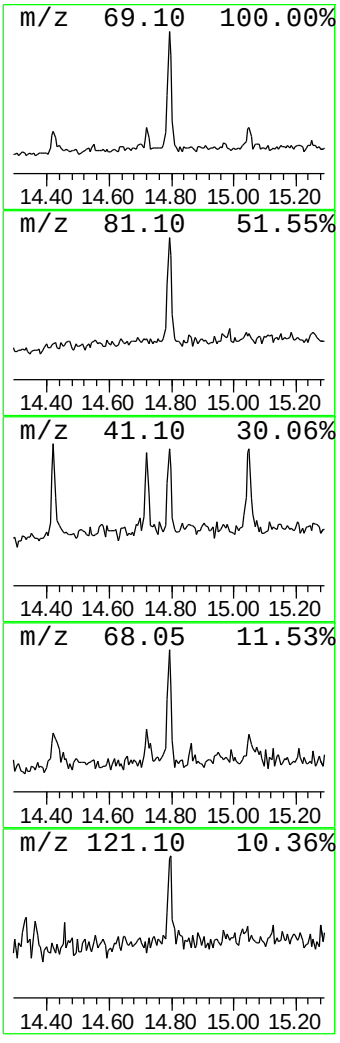
Peak Number 11 Supraene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	2.57 ng	119439	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	80
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
3	Squalene	410	C30H50	000111-02-4	72
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
5	Farnesol isomer a	222	C15H26O	1000108-92-4	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111564.D
Acq On : 18 Dec 2018 2:53
Operator : JU/SJ
Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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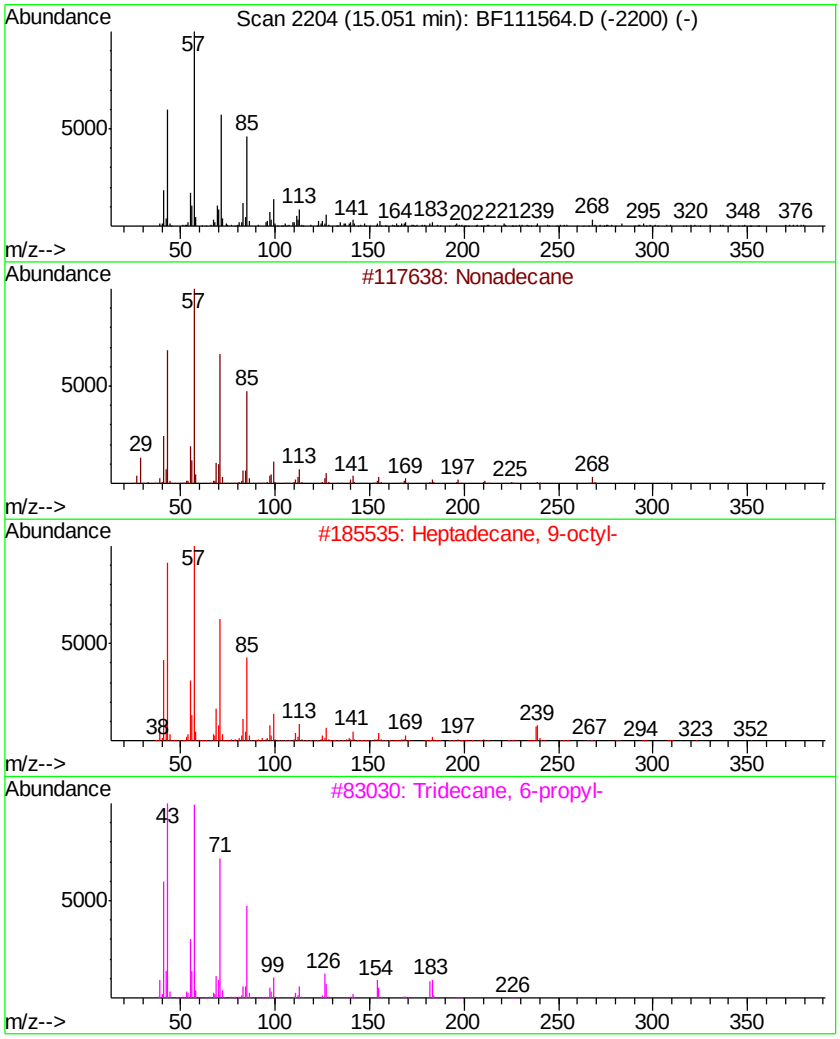
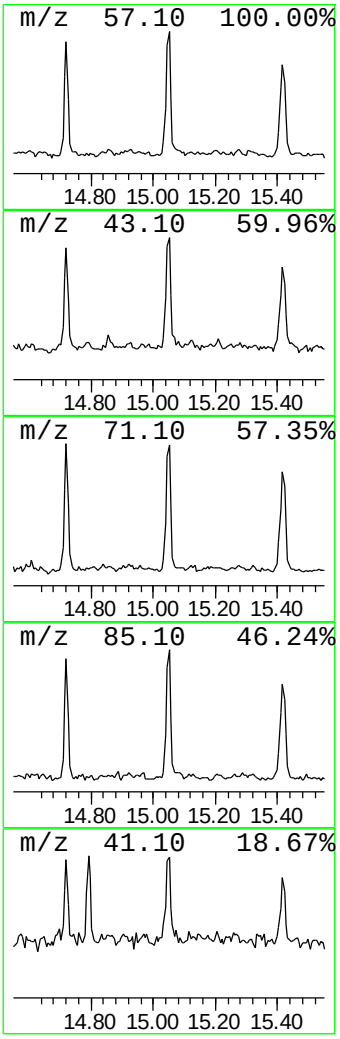
Peak Number 12 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	5.76 ng	267852	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3	Tridecane, 6-propyl-	226	C16H34	055045-10-8	87
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetracosane	338	C24H50	000646-31-1	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121718\
Data File : BF111564.D
Acq On : 18 Dec 2018 2:53
Operator : JU/SJ
Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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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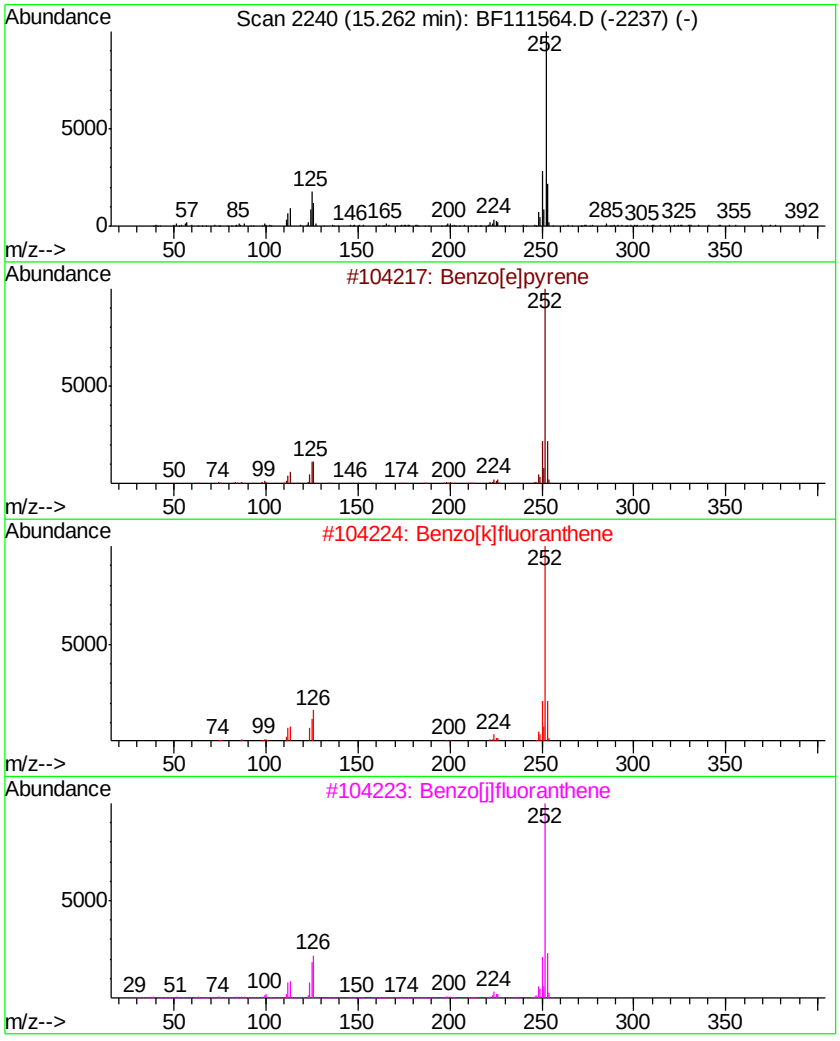
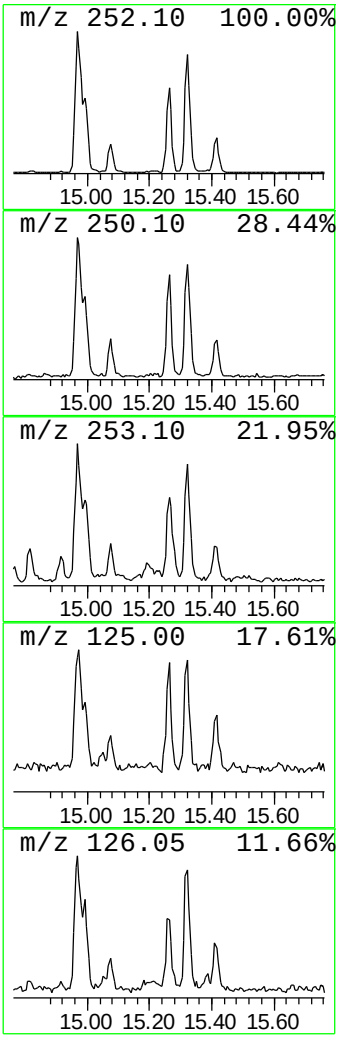
Peak Number 13 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	4.55 ng	211684	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	96
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	93
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Perylene	252	C20H12	000198-55-0	93





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121718\
Data File : BF111564.D
Acq On : 18 Dec 2018 2:53
Operator : JU/SJ
Sample : J6403-53
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-7-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121418.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
unknown3.25	3.25	3.9	ng	157847	1	6.79	813499	20.0
2-Pentanone, 4-hy...	5.00	5.5	ng	223476	1	6.79	813499	20.0
unknown6.57	6.57	86.3	ng	3508710	1	6.79	813499	20.0
n-Hexadecanoic acid	11.84	6.8	ng	395192	4	11.31	1165670	20.0
Octadecanoic acid	12.62	2.2	ng	130457	4	11.31	1165670	20.0
3-Eicosene, (E)-	13.80	5.0	ng	377245	5	13.94	1503210	20.0
Tricosane, 2-methyl-	14.42	3.5	ng	259090	5	13.94	1503210	20.0
Eicosane	14.72	4.3	ng	199362	6	15.39	929596	20.0
Supraene	14.79	2.6	ng	119439	6	15.39	929596	20.0
Nonadecane	15.05	5.8	ng	267852	6	15.39	929596	20.0
Benzo[e]pyrene	15.26	4.5	ng	211684	6	15.39	929596	20.0