LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097556.D
Acq On : 10 Aug 2017 12:05
Operator : SJ/JU
Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

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-BF072517.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	4.522	462	465	485	rBV	108648	233863	10.24%	1.070%
2	4.993	542	545	573	rBV	1438312	2185655	95.74%	10.003%
3	6.069	725	728	742	rBV	1903635	2282947	100.00%	10.448%
4	6.169	742	745	761	rVB	2084334	2214534	97.00%	10.135%
5	6.398	780	784	799	rVB	689112	745931	32.67%	3.414%
6	6.551	806	810	826	rBV	1597017	1632258	71.50%	7.470%
7	6.969	878	881	905	rBV	1356811	1440221	63.09%	6.591%
8	7.681	998	1002	1008	rBV	1001891	985450	43.17%	4.510%
9	7.763	1014	1016	1023	rVB	18039	23349	1.02%	0.107%
10	8.128	1073	1078	1084	rBV	43067	55724	2.44%	0.255%
11	8.298	1101	1107	1110	rBV3	22464	31387	1.37%	0.144%
12	8.386	1118	1122	1125	rVB4	18139	24887	1.09%	0.114%
13	8.657	1165	1168	1172	rVB4	25371	27302	1.20%	0.125%
14	8.698	1172	1175	1176	rBV	23731	23362	1.02%	0.107%
15	8.722	1176	1179	1181	rVV	84311	72747	3.19%	0.333%
16	8.757	1181	1185	1194	rVB	2207290	2039373	89.33%	9.333%
17	8.857	1198	1202	1207	rVV	49716	61163	2.68%	0.280%
18	9.033	1224	1232	1235	rBV8	25469	58934	2.58%	0.270%
19	9.104	1240	1244	1246	rVV3	29982	49658	2.18%	0.227%
20	9.128	1246	1248	1251	rVV3	41417	36205	1.59%	0.166%
21	9.163	1251	1254	1262	rVV2	245785	317582	13.91%	1.453%
22	9.381	1288	1291	1294	rBV	95012	84507	3.70%	0.387%
23	9.422	1294	1298	1303	rVV	982114	893158	39.12%	4.088%
24	9.539	1312	1318	1326	rBV4	28355	52604	2.30%	0.241%
25	9.610	1326	1330	1332	rBV2	33057	48059	2.11%	0.220%
26	9.639	1332	1335	1338	rVV3	61862	67125	2.94%	0.307%
27	9.675	1338	1341	1343	rVV2	34176	43852	1.92%	0.201%
28	9.698	1343	1345	1349	rVB	76150	64607	2.83%	0.296%
29	9.739	1349	1352	1357	rVB3	29878	39569	1.73%	0.181%
30	9.875	1370	1375	1379	rBV	117695	116336	5.10%	0.532%
31	10.098	1408	1413	1415	rBV	173726	195708	8.57%	0.896%
32	10.145	1419	1421	1424	rVB3	37795	28395	1.24%	0.130%
33	10.180	1424	1427	1428	rBV2	29741	27985	1.23%	0.128%
34	10.210	1428	1432	1437	rBV	913486	893247	39.13%	4.088%

LSC Area Percent Report

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Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

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

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Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.357	1449	1457	1462	rBV	260635	431709	18.91%	1.976%
36	10.539	1485	1488	1491	rBV2	64666	71850	3.15%	0.329%
37	10.569	1491	1493	1495	rVB2	33177	29087	1.27%	0.133%
38	10.669	1508	1510	1514	rVB4	26685	24720	1.08%	0.113%
39	10.792	1528	1531	1533	rVV	122015	110786	4.85%	0.507%
40	10.822	1533	1536	1542	rVB	189939	195113	8.55%	0.893%
41	10.898	1545	1549	1553	rBV	701507	695297	30.46%	3.182%
42	10.969	1559	1561	1566	rVB4	23427	26172	1.15%	0.120%
43	11.169	1592	1595	1598	rVB	46944	45442	1.99%	0.208%
44	11.216	1600	1603	1606	rBV	87679	72981	3.20%	0.334%
45	11.510	1650	1653	1656	rBV3	26069	30455	1.33%	0.139%
46	11.622	1669	1672	1676	rVB	58633	65218	2.86%	0.298%
47	11.898	1717	1719	1724	rVB2	27114	30461	1.33%	0.139%
48	11.951	1724	1728	1732	rVV3	20705	30294	1.33%	0.139%
49	12.004	1734	1737	1740	rVB	44694	39254	1.72%	0.180%
50	12.322	1788	1791	1794	rBV	31737	27833	1.22%	0.127%
51	12.474	1813	1817	1821	rBV	1305314	1184408	51.88%	5.421%
52	12.969	1896	1901	1907	rBV	534912	561042	24.58%	2.568%
53	13.398	1967	1974	1982	rBV2	38356	70014	3.07%	0.320%
54	13.521	1991	1995	2003	rBV	485676	515823	22.59%	2.361%
55	14.857	2218	2222	2235	rBV	406167	494480	21.66%	2.263%

Sum of corrected areas: 21850123

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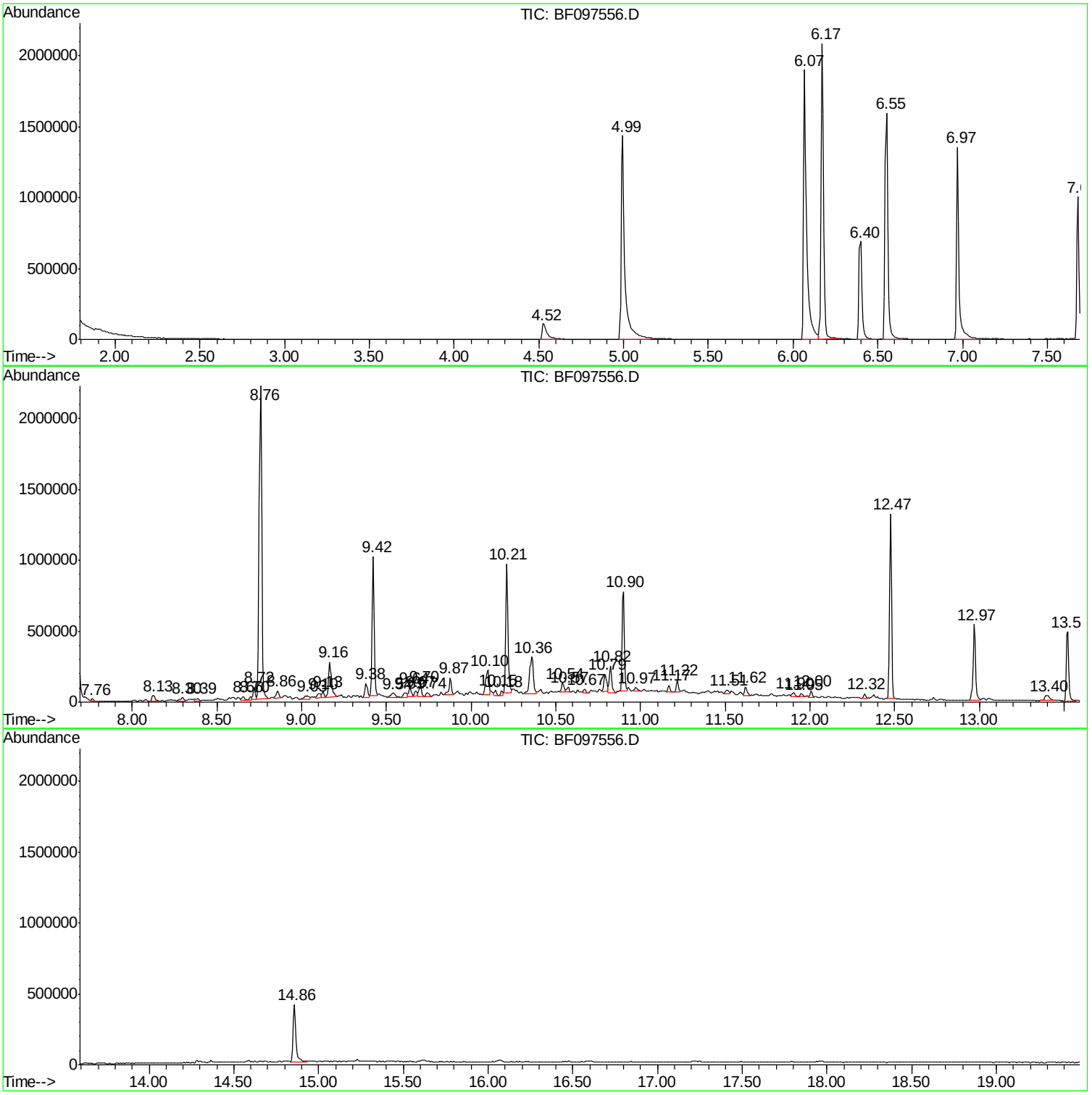
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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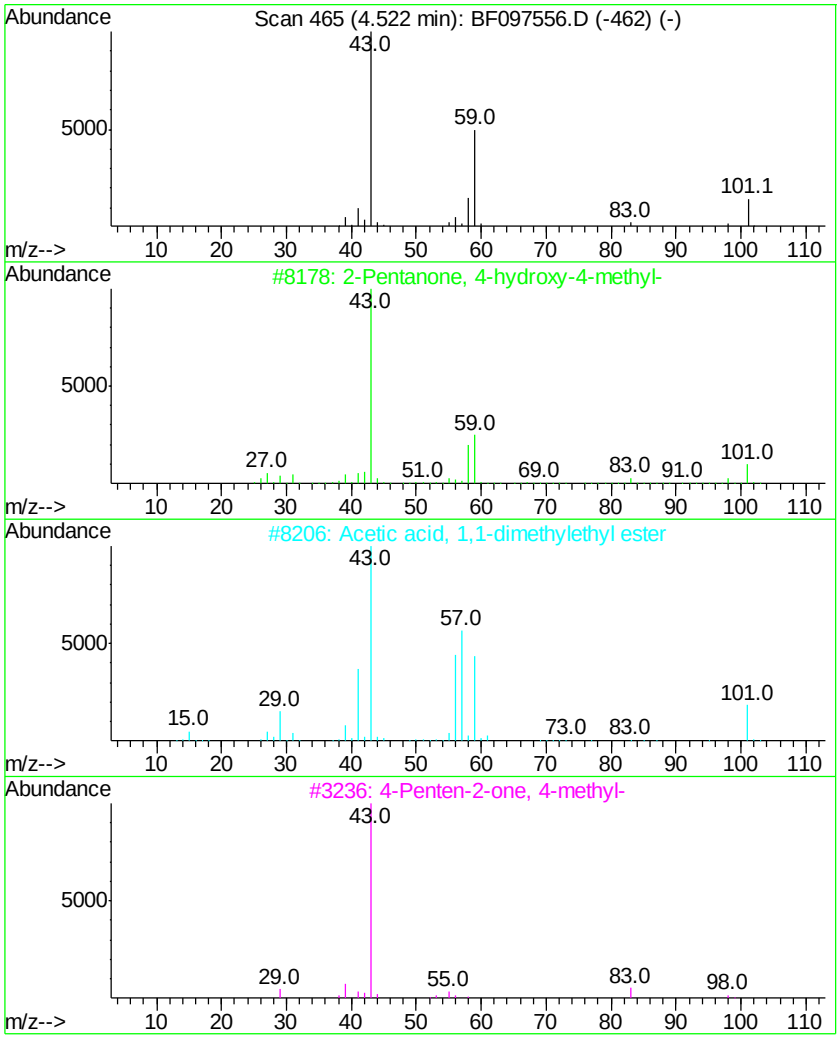
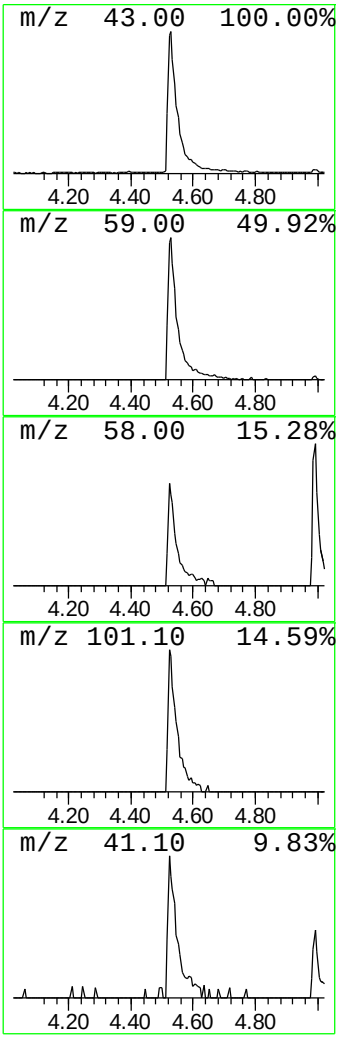
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	6.27 ng	233863	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Library Search Compound Report

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Acq On : 10 Aug 2017 12:05
Operator : SJ/JU
Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

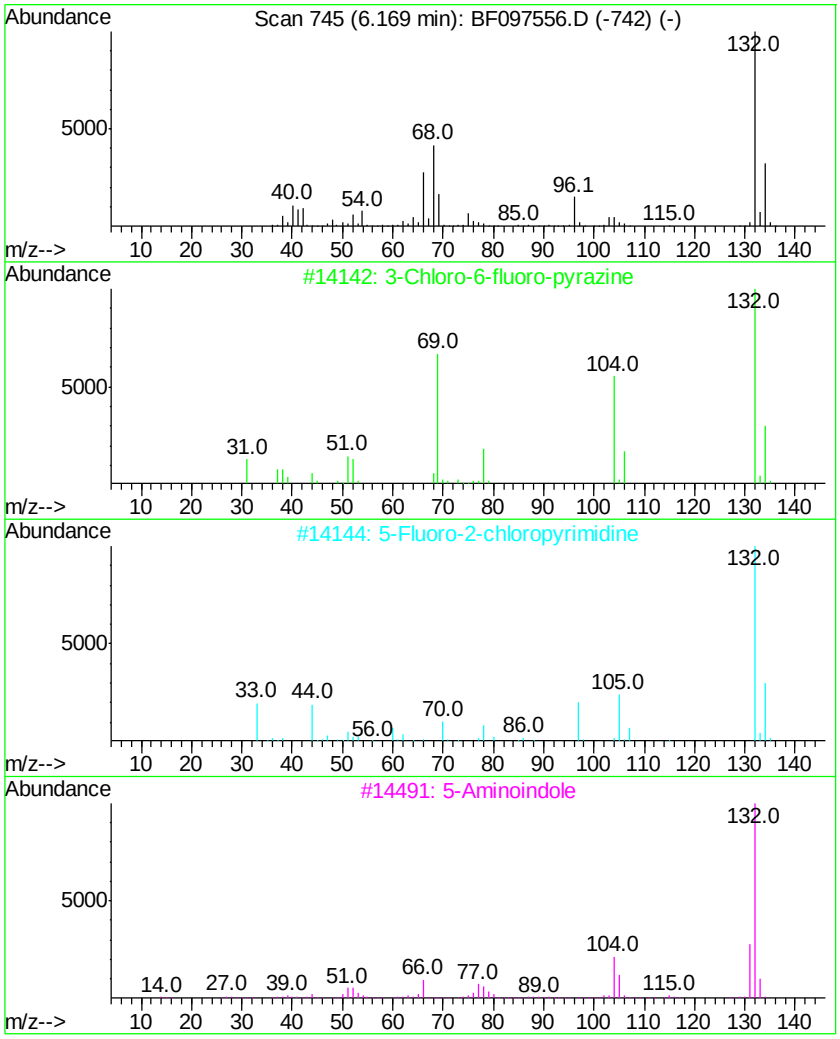
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

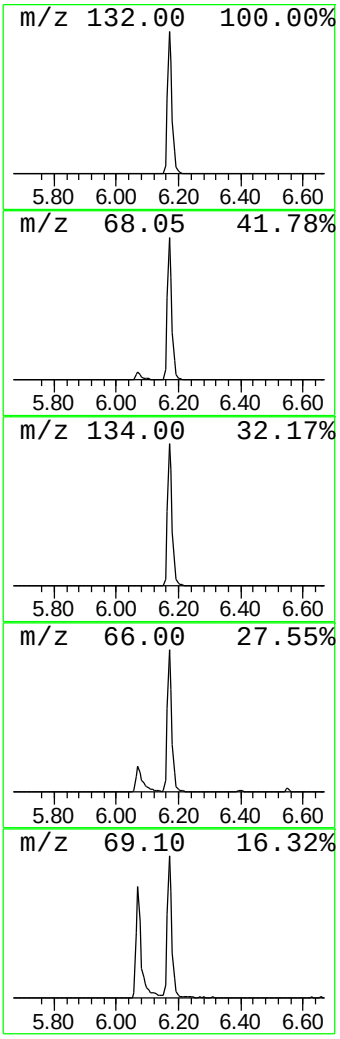
****

Peak Number 2 unknown6.17 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.17	59.38 ng	2214530	1,4-Dichlorobenzene-d4	6.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Sample : I4623-12
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ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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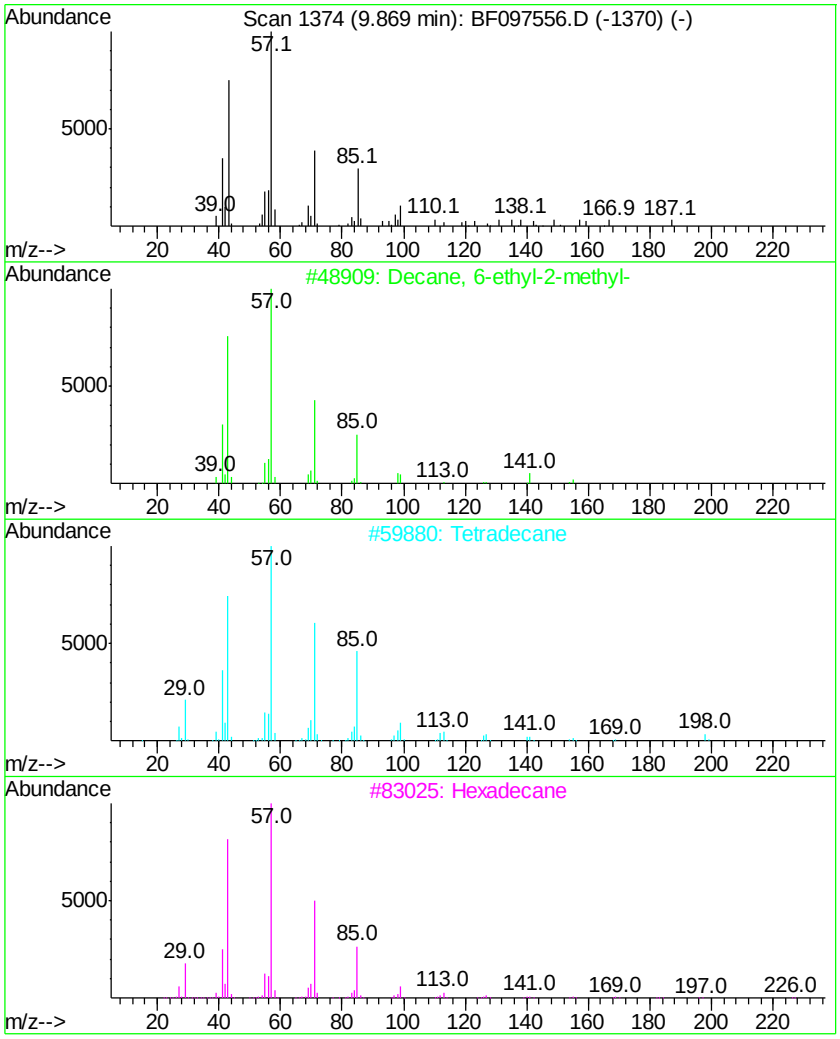
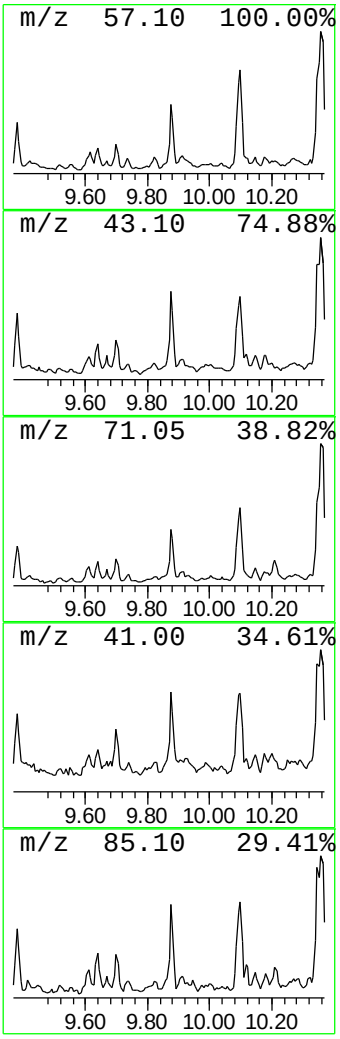
****

Peak Number 4 Decane, 6-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	2.61 ng	116336	Acenaphthene-d10	9.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	78
2	Tetradecane	198	C14H30	000629-59-4	78
3	Hexadecane	226	C16H34	000544-76-3	72
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	64
5	Tetracosane	338	C24H50	000646-31-1	64





Library Search Compound Report

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Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

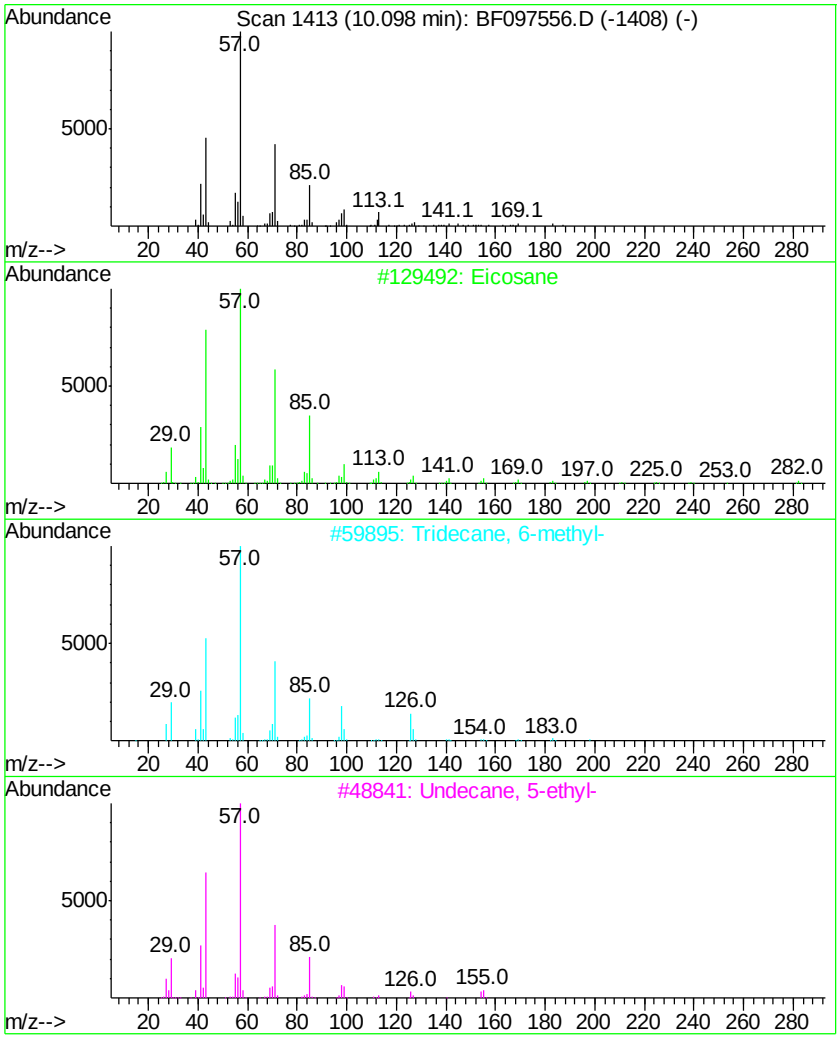
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

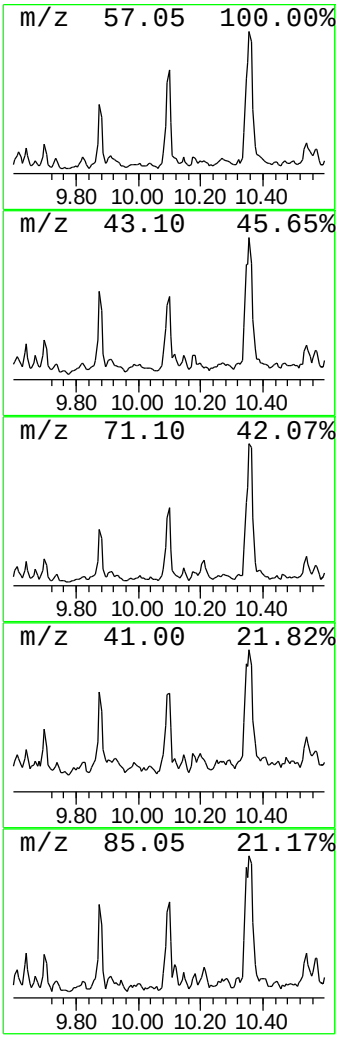
****

Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	4.38 ng	195708	Acenaphthene-d10	9.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	80
2	Tridecane, 6-methyl-	198	C14H30	013287-21-3	78
3	Undecane, 5-ethyl-	184	C13H28	017453-94-0	78
4	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	72
5	Tetracosane	338	C24H50	000646-31-1	72





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Sample : I4623-12
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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TIC Library : C:\DATABASE\NIST11.L
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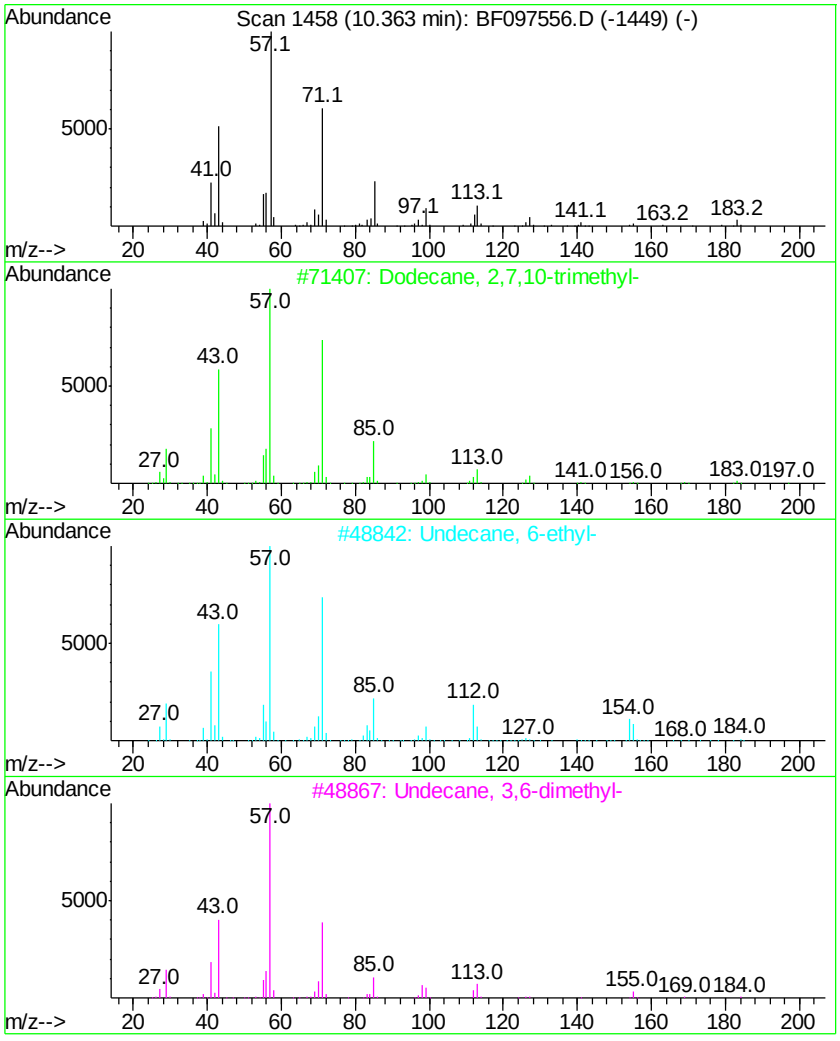
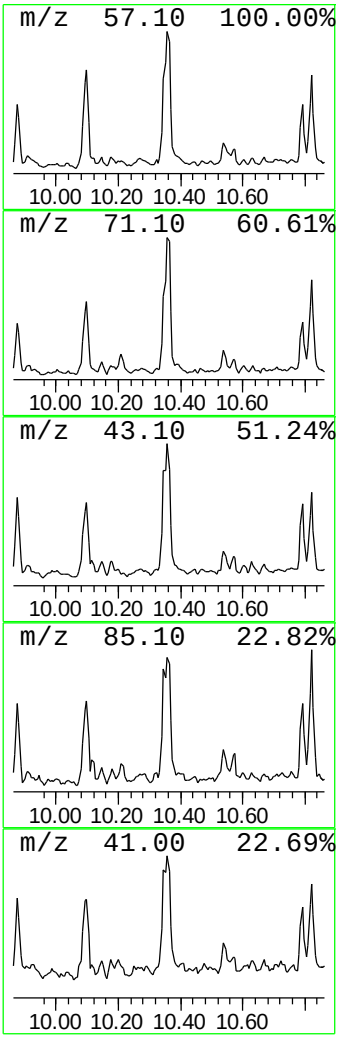
****

Peak Number 6 Dodecane, 2,7,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	12.42 ng	431709	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	90
2	Undecane, 6-ethyl-	184	C13H28	017312-60-6	81
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	74
4	Hexadecane	226	C16H34	000544-76-3	72
5	Tridecane, 5-propyl-	226	C16H34	055045-11-9	64





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ClientSampleId : TEC-S2COMP

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TIC Library : C:\DATABASE\NIST11.L
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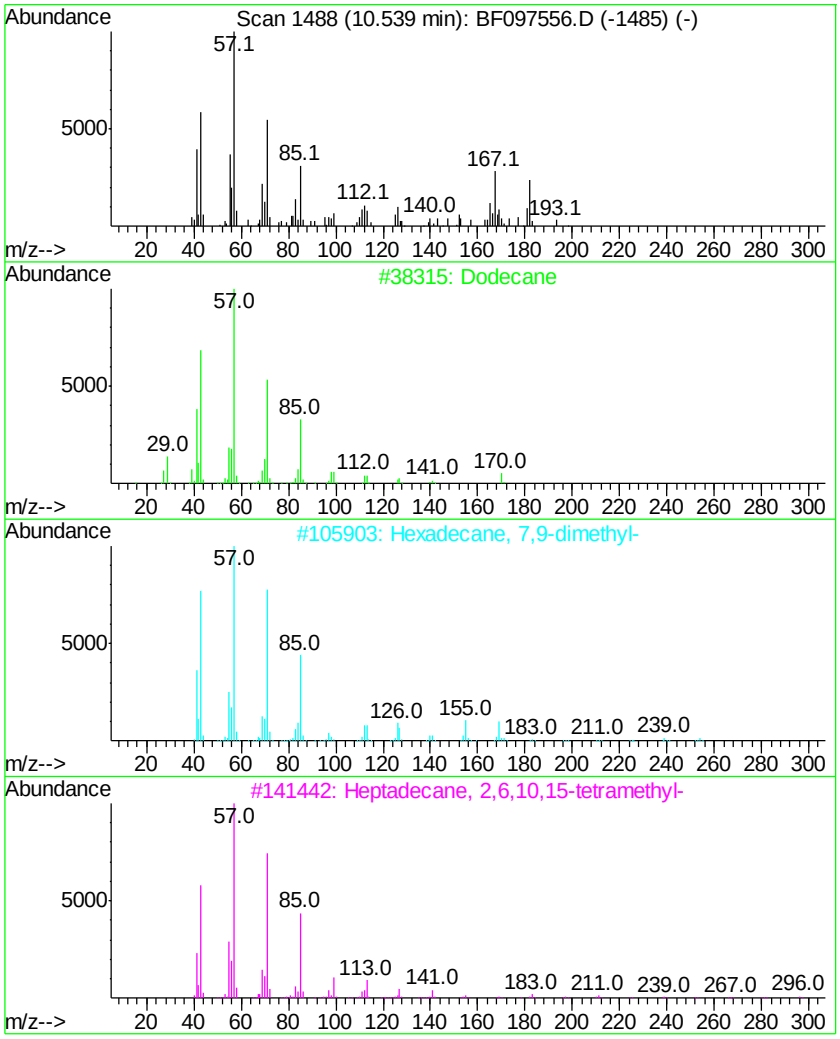
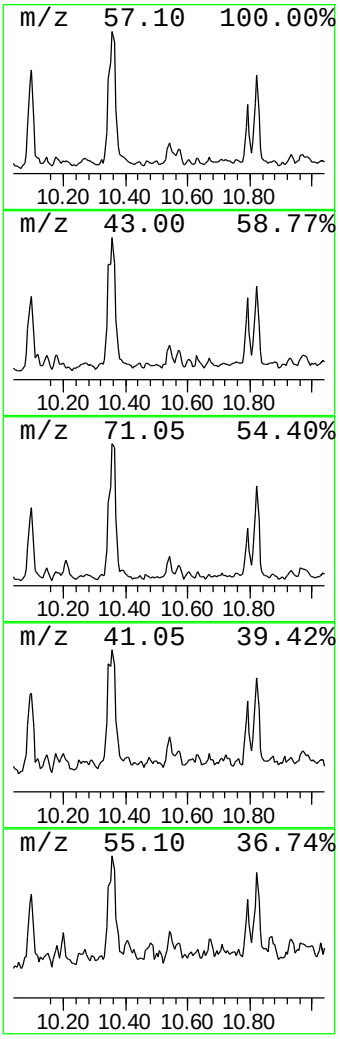
Peak Number 7 unknown10.54 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	2.07 ng	71850	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	49
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	47
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	38
4	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	38
5	Undecane, 6-ethyl-	184	C13H28	017312-60-6	35





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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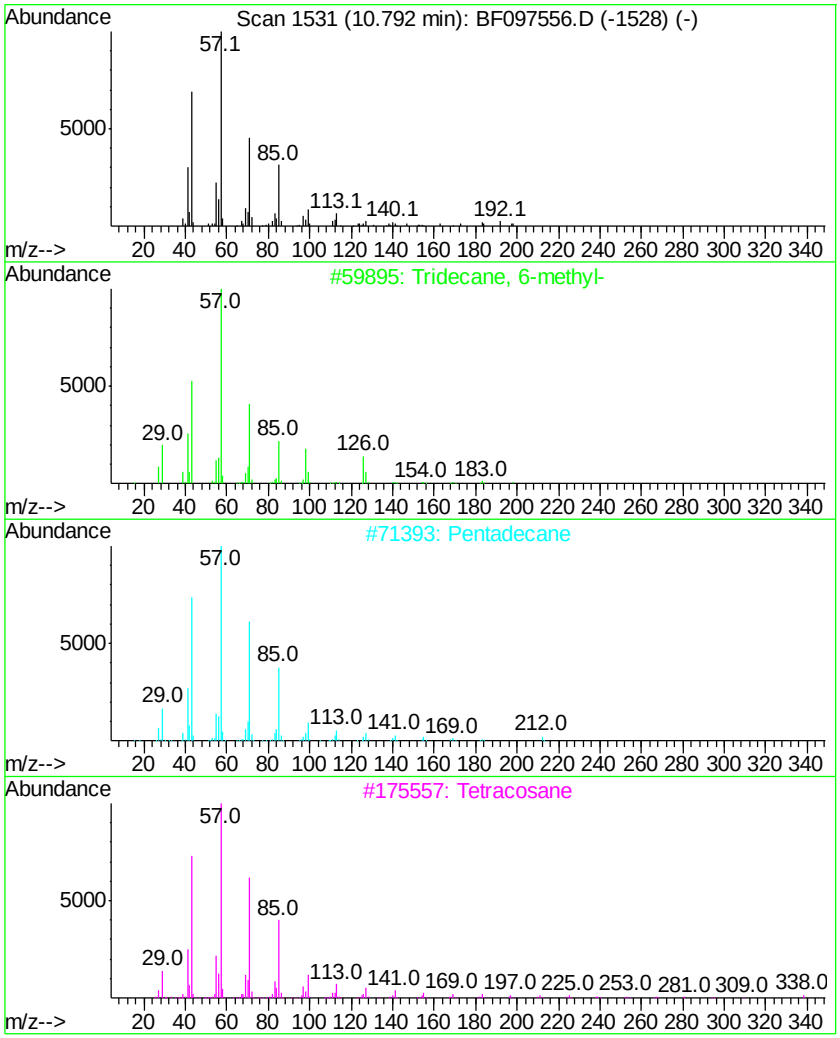
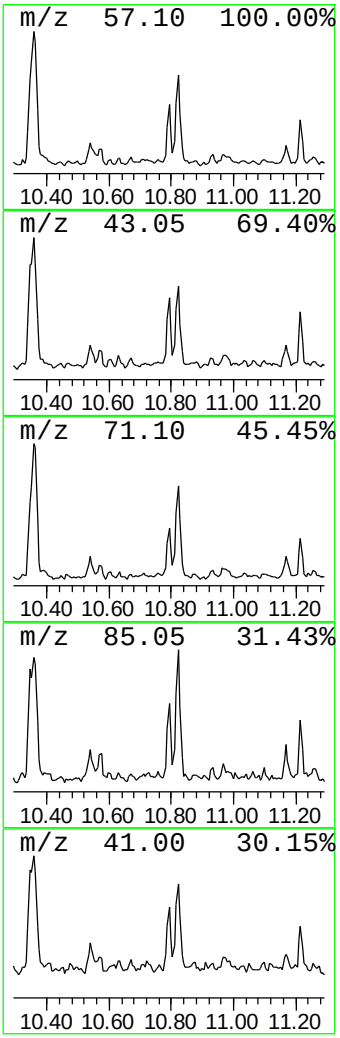
Peak Number 8 Tridecane, 6-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	3.19 ng	110786	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 6-methyl-	198	C14H30	013287-21-3	81
2	Pentadecane	212	C15H32	000629-62-9	80
3	Tetracosane	338	C24H50	000646-31-1	80
4	Hexadecane	226	C16H34	000544-76-3	80
5	Tridecane	184	C13H28	000629-50-5	74





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Sample : I4623-12
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Instrument : BNA_F
ClientSampleId : TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
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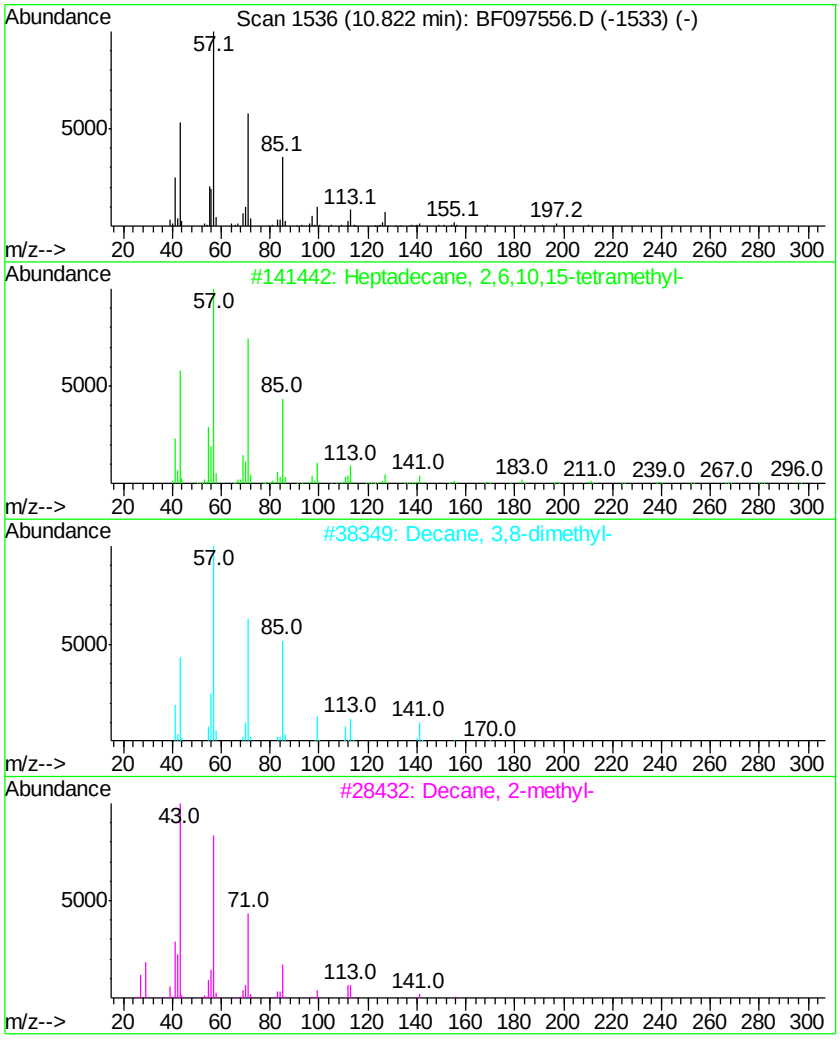
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

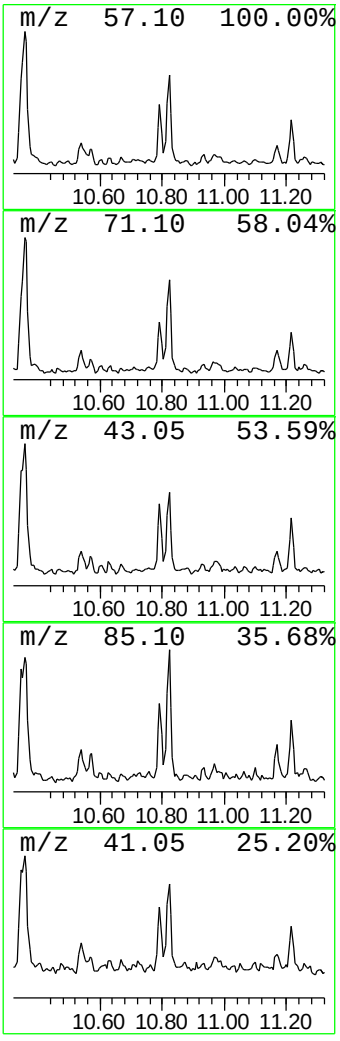
****

Peak Number 9 Heptadecane, 2,6,10,15-tetr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	5.61 ng	195113	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	78
3	Decane, 2-methyl-	156	C11H24	006975-98-0	72
4	Heptacosane	380	C27H56	000593-49-7	72
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64





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Data File : BF097556.D
Acq On : 10 Aug 2017 12:05
Operator : SJ/JU
Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

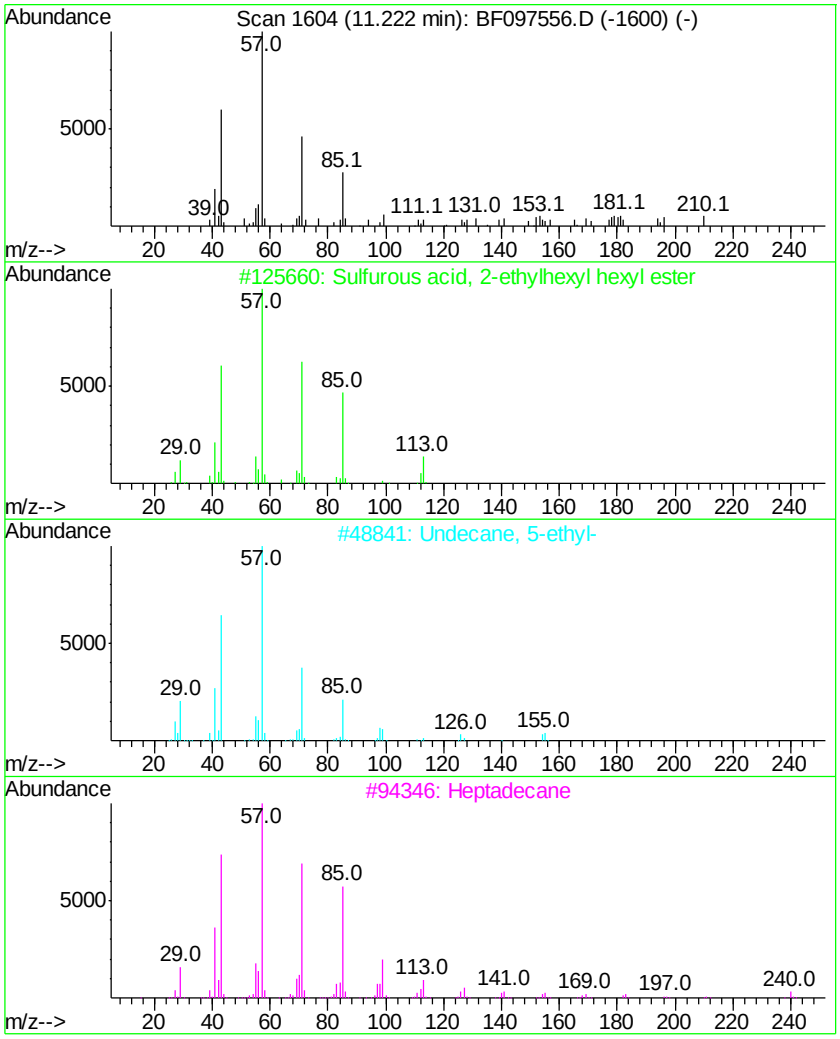
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

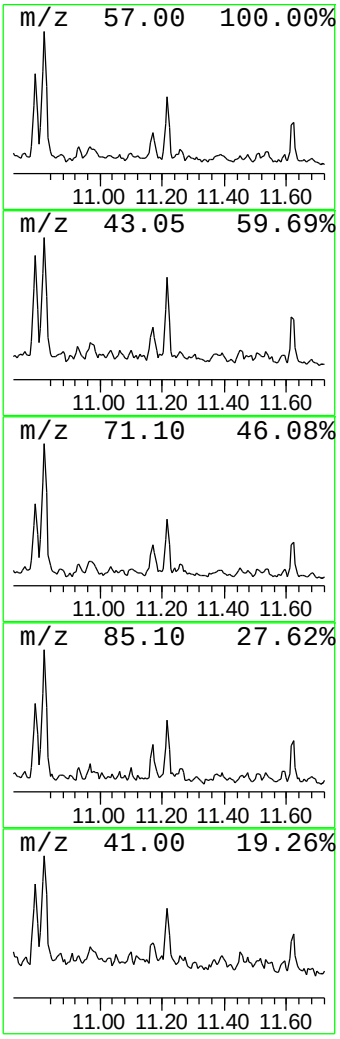
****

Peak Number 10 Sulfurous acid, 2-ethylhexy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	2.10 ng	72981	Phenanthrene-d10	10.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	80
2	Undecane, 5-ethyl-	184	C13H28	017453-94-0	78
3	Heptadecane	240	C17H36	000629-78-7	78
4	Octacosane	394	C28H58	000630-02-4	78
5	Pentadecane	212	C15H32	000629-62-9	72





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Operator : SJ/JU
Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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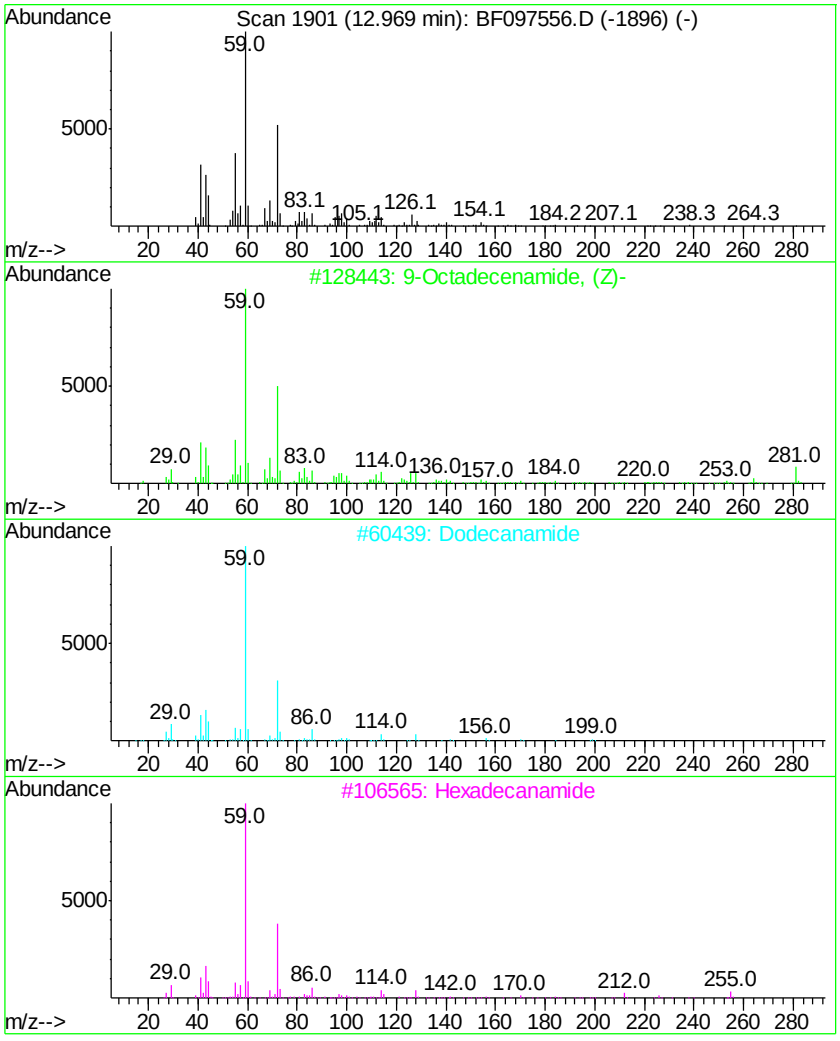
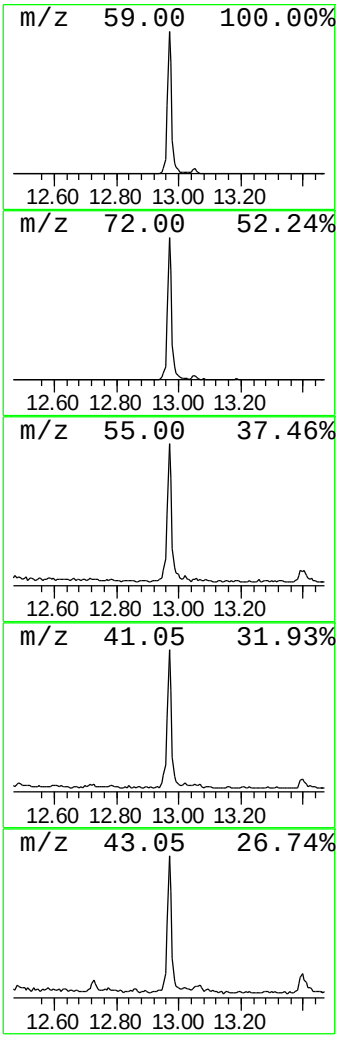
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	21.75 ng	561042	Chrysene-d12	13.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Dodecanamide	199	C12H25NO	001120-16-7	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	59
4	Nonanamide	157	C9H19NO	001120-07-6	53
5	2-Pentanol, 3-chloro-2-methyl-	136	C6H13ClO	074685-49-7	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080917\
Data File : BF097556.D
Acq On : 10 Aug 2017 12:05
Operator : SJ/JU
Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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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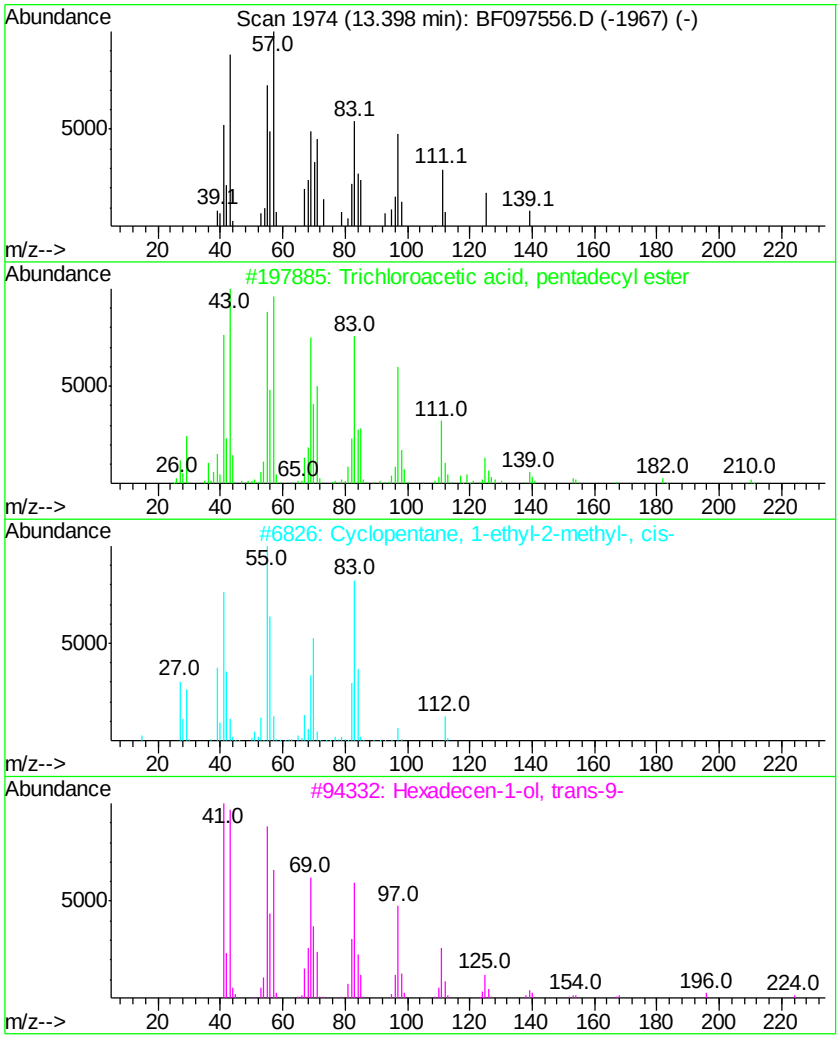
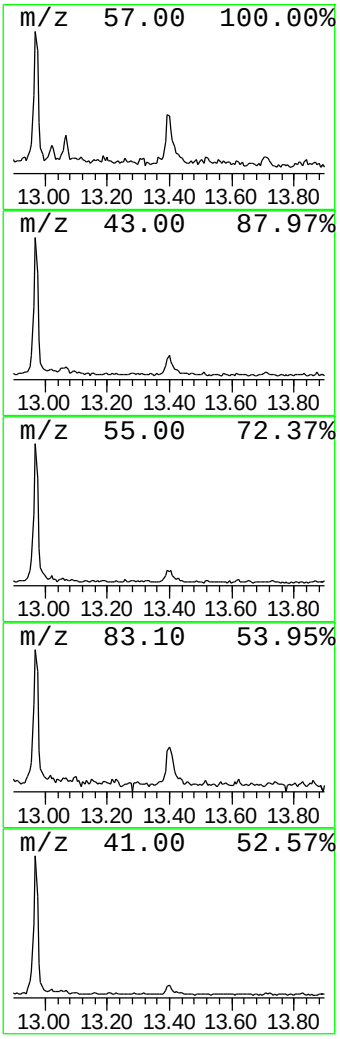
Peak Number 12 Trichloroacetic acid, penta... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.71 ng	70014	Chrysene-d12	13.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81
2	Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	80
3	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	80
4	Cetene	224	C16H32	000629-73-2	80
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080917\
Data File : BF097556.D
Acq On : 10 Aug 2017 12:05
Operator : SJ/JU
Sample : I4623-12
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TEC-S2COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.52	6.3	ng	233863	1	6.40	745931	20.0
unknown6.17	6.17	59.4	ng	2214530	1	6.40	745931	20.0
Decane, 6-ethyl-2...	9.87	2.6	ng	116336	3	9.42	893158	20.0
Eicosane	10.10	4.4	ng	195708	3	9.42	893158	20.0
Dodecane, 2,7,10-...	10.36	12.4	ng	431709	4	10.90	695297	20.0
unknown10.54	10.54	2.1	ng	71850	4	10.90	695297	20.0
Tridecane, 6-methyl-	10.79	3.2	ng	110786	4	10.90	695297	20.0
Heptadecane, 2,6,...	10.82	5.6	ng	195113	4	10.90	695297	20.0
Sulfurous acid, 2...	11.22	2.1	ng	72981	4	10.90	695297	20.0
9-Octadecenamide,...	12.97	21.8	ng	561042	5	13.52	515823	20.0
Trichloroacetic a...	13.40	2.7	ng	70014	5	13.52	515823	20.0