LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101215.D
Acq On : 7 Dec 2017 19:46
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

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-BF113017.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	5.069	504	507	521	rBB	54137	73071	6.63%	0.679%
2	5.463	570	574	588	rBV	997933	1038413	94.18%	9.653%
3	6.481	742	747	761	rVB	1067709	1049755	95.21%	9.758%
4	6.616	765	770	773	rBV	1238531	1067362	96.80%	9.922%
5	6.839	805	808	812	rBV	306419	256690	23.28%	2.386%
6	6.998	831	835	838	rBV	1007692	845251	76.66%	7.857%
7	7.410	900	905	908	rBV	643186	581571	52.74%	5.406%
8	8.122	1023	1026	1034	rBV	333898	305946	27.75%	2.844%
9	9.198	1205	1209	1212	rBV	1250740	1102609	100.00%	10.249%
10	9.592	1273	1276	1279	rBV	133659	95801	8.69%	0.891%
11	9.798	1308	1311	1316	rBB	23958	20596	1.87%	0.191%
12	9.880	1321	1325	1329	rVV	345367	286939	26.02%	2.667%
13	9.916	1329	1331	1333	rVB	16799	12321	1.12%	0.115%
14	10.298	1393	1396	1399	rVB	29539	23966	2.17%	0.223%
15	10.675	1456	1460	1463	rBV	640542	530227	48.09%	4.929%
16	10.775	1474	1477	1487	rBV	26315	27960	2.54%	0.260%
17	11.374	1575	1579	1581	rBV	323480	273143	24.77%	2.539%
18	11.398	1581	1583	1586	rVV	118457	89310	8.10%	0.830%
19	11.451	1586	1592	1595	rVV	24262	20881	1.89%	0.194%
20	11.892	1661	1667	1672	rBV3	21082	39988	3.63%	0.372%
21	11.992	1680	1684	1686	rBV2	18093	21744	1.97%	0.202%
22	12.592	1782	1786	1789	rBV	148076	135026	12.25%	1.255%
23	12.774	1813	1817	1819	rVB	15310	13769	1.25%	0.128%
24	12.821	1822	1825	1828	rVB	134827	111712	10.13%	1.038%
25	12.957	1844	1848	1851	rBV	918579	885150	80.28%	8.228%
26	13.039	1858	1862	1866	rBV3	8991	13706	1.24%	0.127%
27	13.151	1874	1881	1884	rBV	21420	26261	2.38%	0.244%
28	13.216	1888	1892	1894	rBV	20497	17862	1.62%	0.166%
29	13.251	1894	1898	1900	rBV3	14608	16657	1.51%	0.155%
30	13.433	1924	1929	1933	rBV	134488	171819	15.58%	1.597%
31	13.504	1940	1941	1947	rVB2	17005	16745	1.52%	0.156%
32	13.768	1983	1986	1988	rBV2	14251	15041	1.36%	0.140%
33	13.839	1993	1998	2002	rVV3	68543	76219	6.91%	0.709%
34	13.986	2019	2023	2024	rBV4	14218	16468	1.49%	0.153%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

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-BF113017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.021	2024	2029	2032	rVV2	315304	334950	30.38%	3.114%
36	14.045	2032	2033	2036	rVB	51599	39792	3.61%	0.370%
37	14.115	2042	2045	2052	rBV3	28196	53866	4.89%	0.501%
38	14.374	2085	2089	2090	rBV4	11163	13627	1.24%	0.127%
39	14.762	2152	2155	2160	rVB3	29271	38229	3.47%	0.355%
40	14.851	2167	2170	2178	rVB	66801	78291	7.10%	0.728%
41	15.068	2204	2207	2211	rBV	41073	69210	6.28%	0.643%
42	15.180	2223	2226	2229	rBV3	17138	19016	1.72%	0.177%
43	15.374	2256	2259	2264	rVB	27994	35638	3.23%	0.331%
44	15.439	2266	2270	2275	rVB	39319	47930	4.35%	0.446%
45	15.504	2276	2281	2286	rBV	162331	208135	18.88%	1.935%
46	15.733	2317	2320	2328	rVB4	30073	47821	4.34%	0.445%
47	16.304	2412	2417	2424	rBV3	36210	77952	7.07%	0.725%
48	16.998	2528	2535	2545	rVB6	60304	159081	14.43%	1.479%
49	17.845	2672	2679	2689	rBV5	43048	118251	10.72%	1.099%
50	18.892	2848	2857	2867	rVB4	34368	135968	12.33%	1.264%

Sum of corrected areas: 10757736

LSC Report - Integrated Chromatogram

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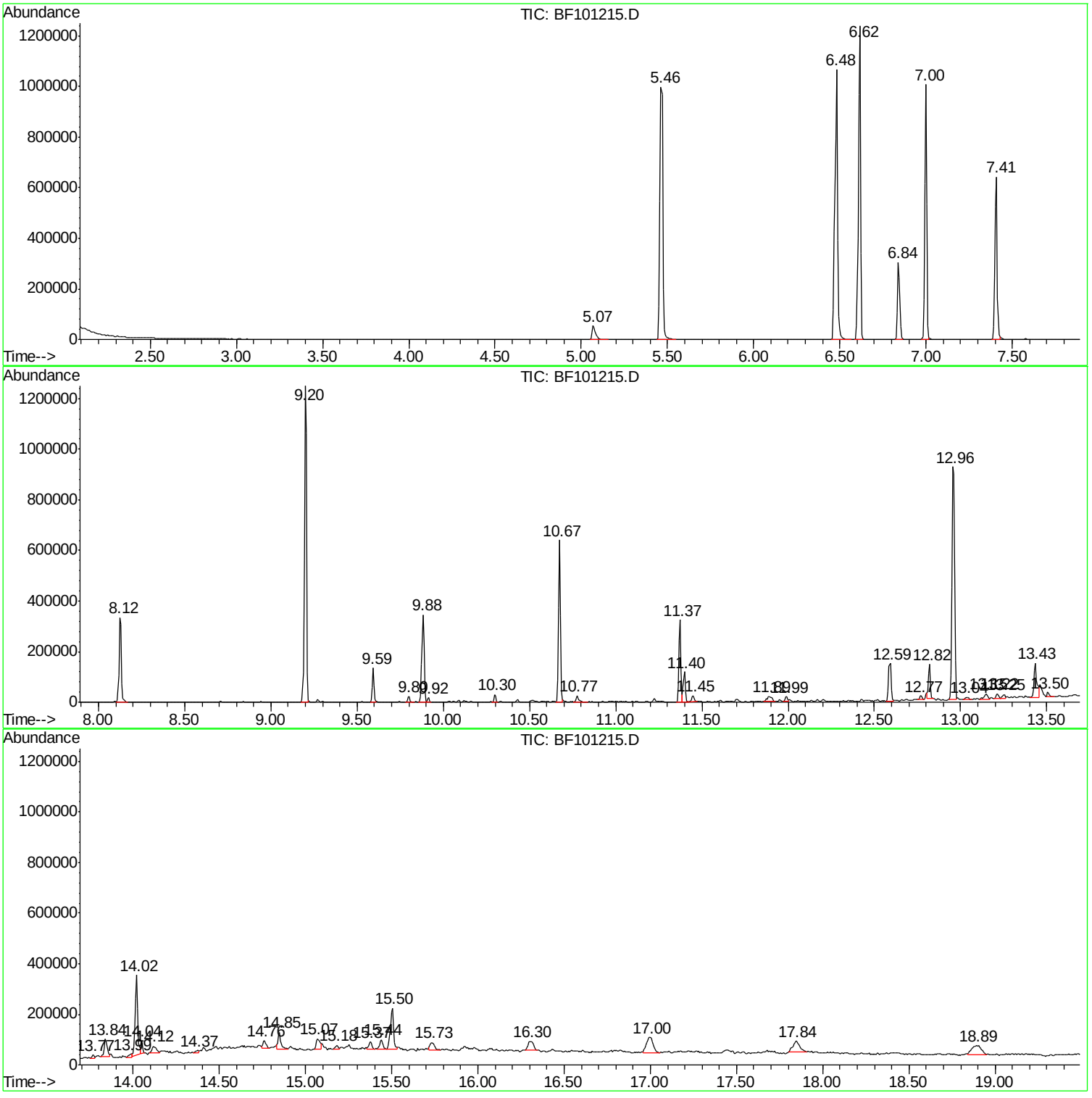
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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Data File : BF101215.D
Acq On : 7 Dec 2017 19:46
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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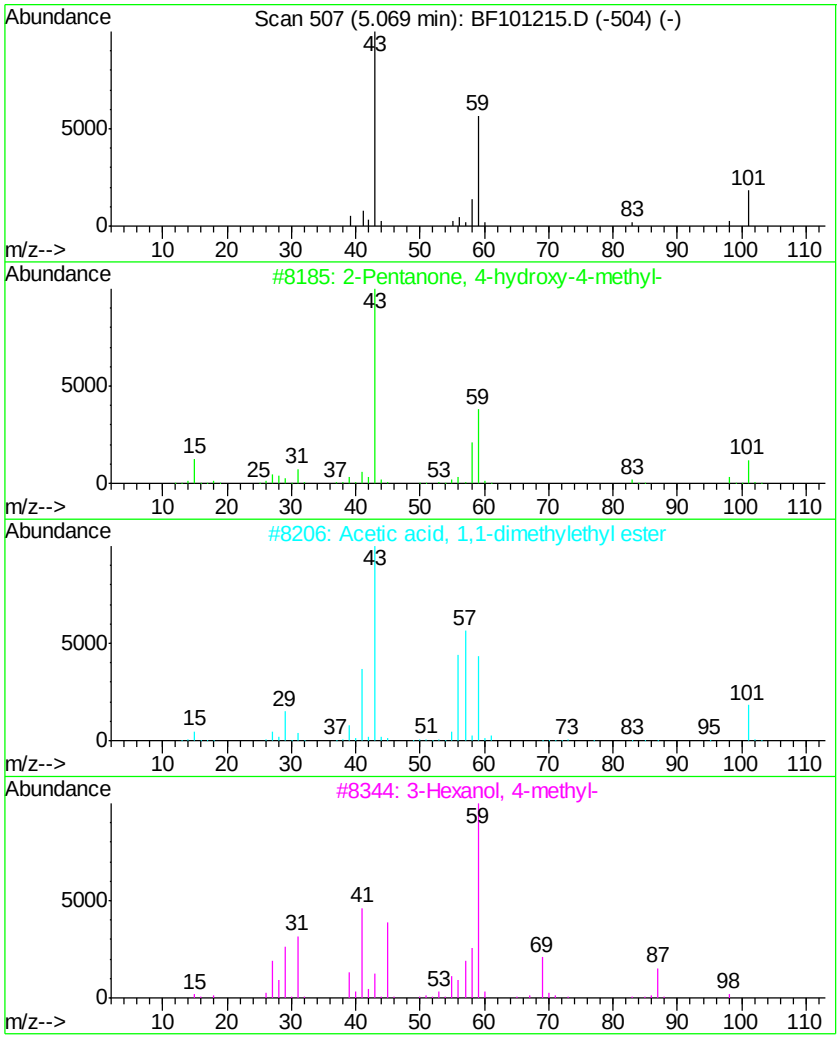
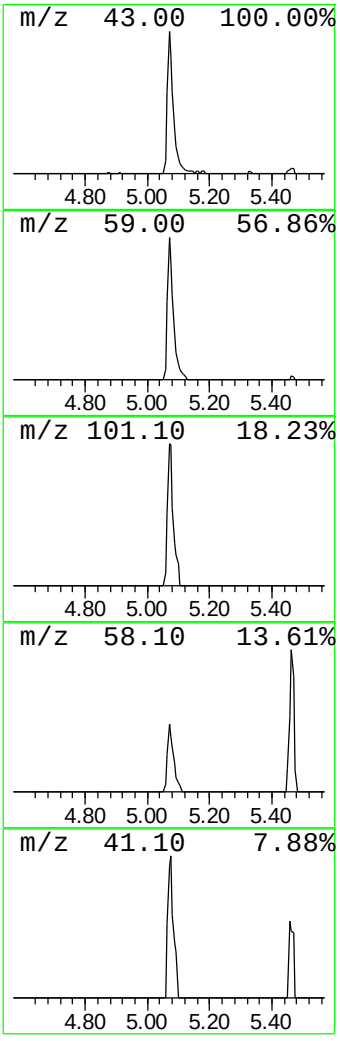
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	5.69 ng	73071	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Pentanol	88	C5H12O	000584-02-1	9





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Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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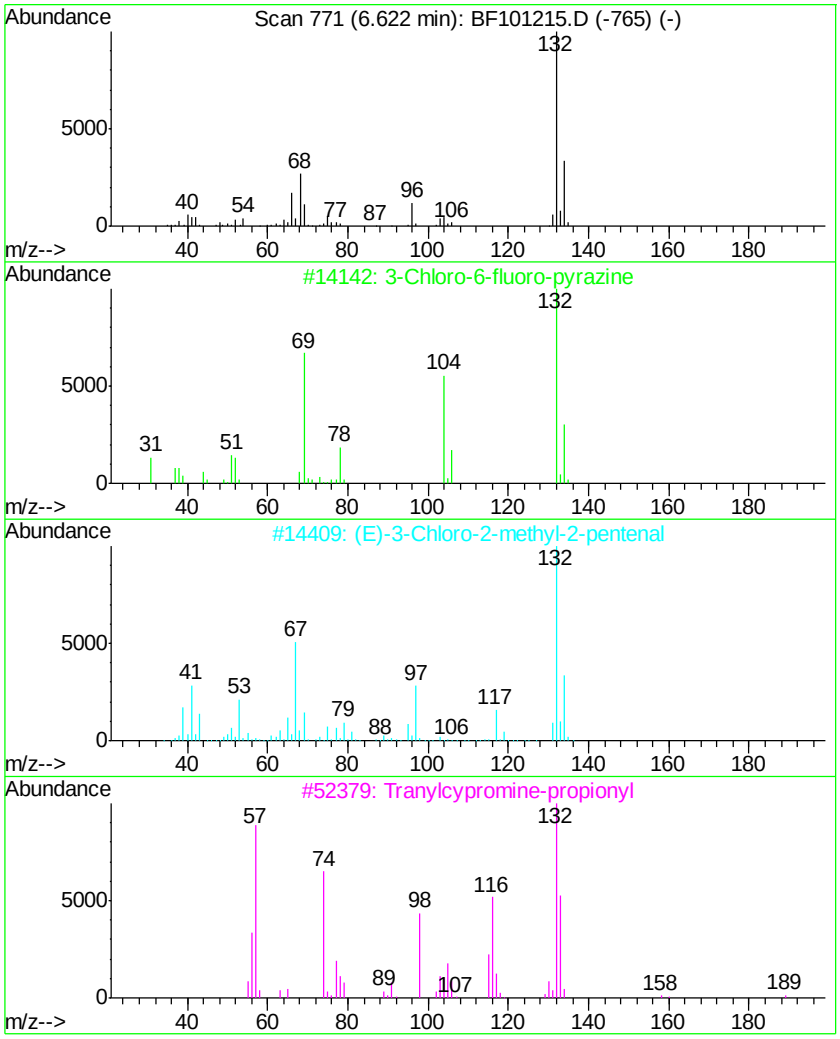
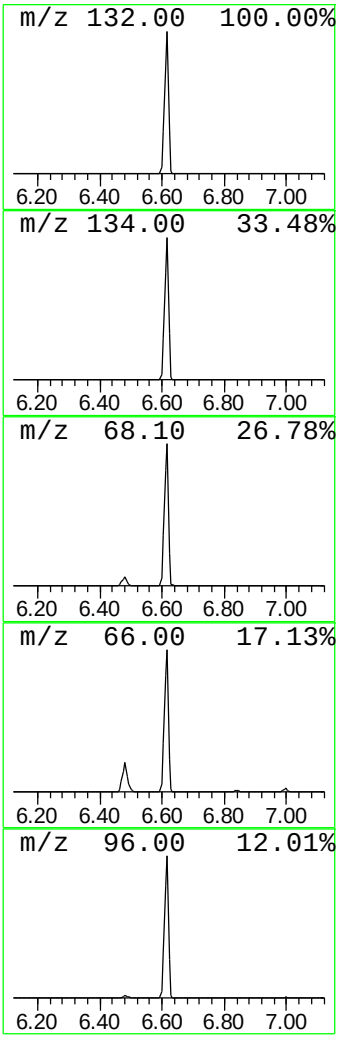
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	83.16 ng	1067360	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101215.D
Acq On : 7 Dec 2017 19:46
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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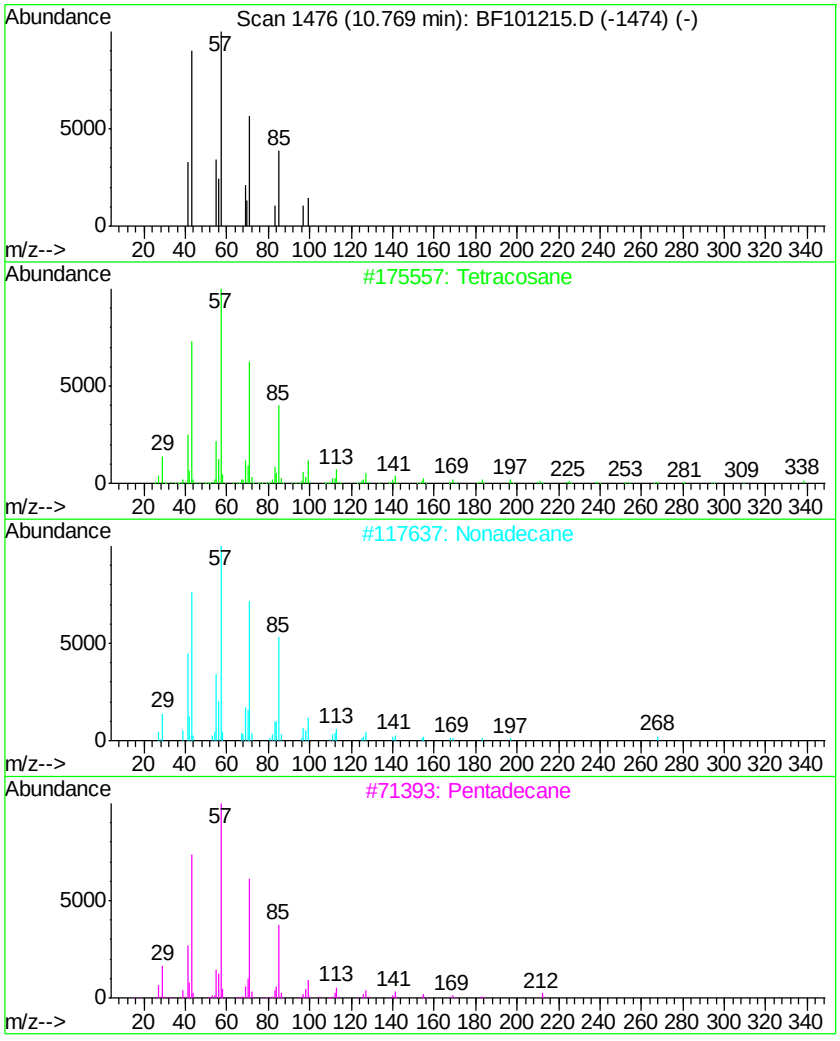
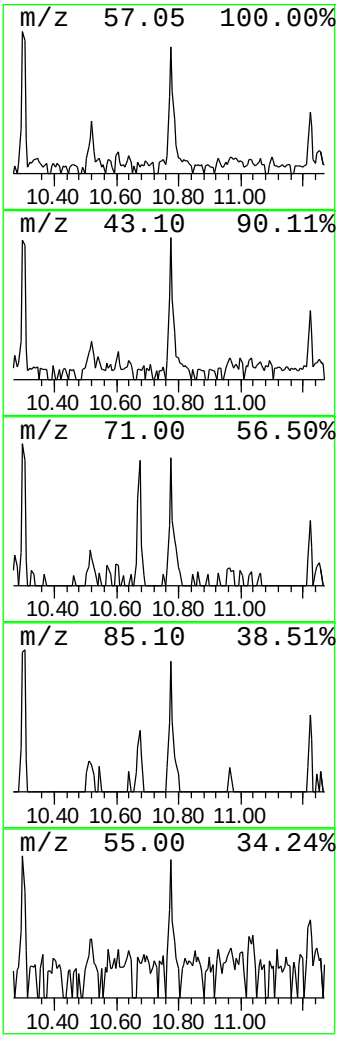
Peak Number 4 Tetracosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.77	2.05 ng	27960	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Nonadecane	268	C19H40	000629-92-5	90
3	Pentadecane	212	C15H32	000629-62-9	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane	282	C20H42	000112-95-8	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
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Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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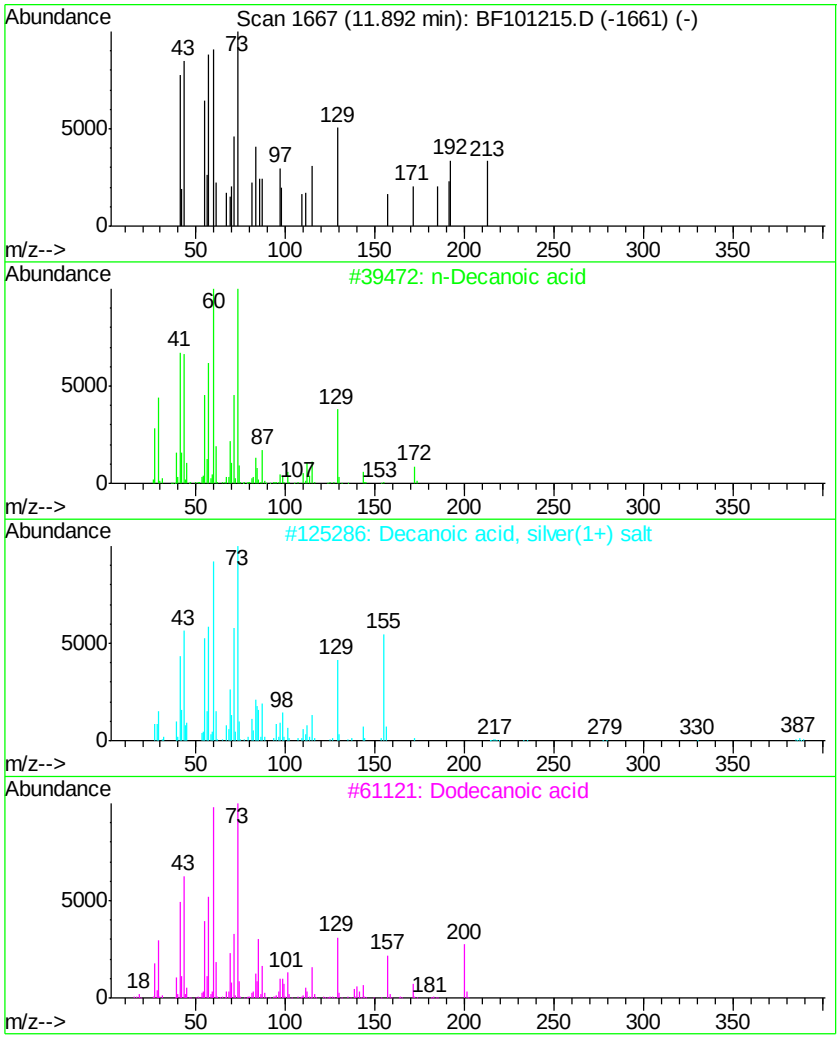
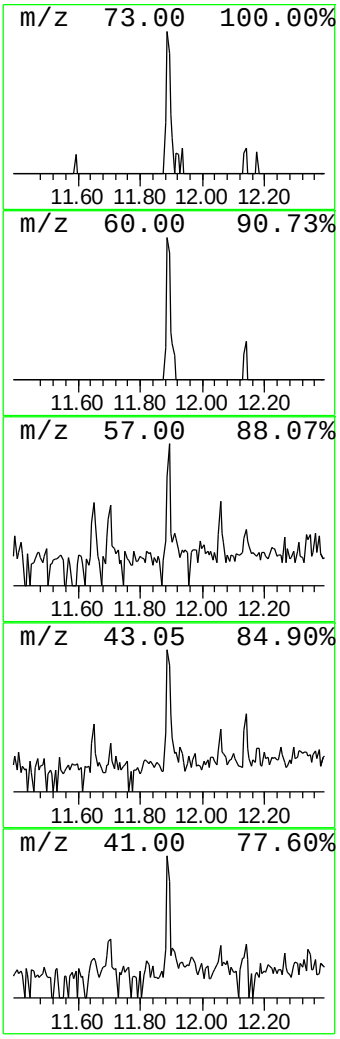
Peak Number 5 unknown11.89 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	2.93 ng	39988	Phenanthrene-d10	11.37

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	38
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	38
3	Dodecanoic acid	200	C12H24O2	000143-07-7	37
4	Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	35
5	Undecanoic acid	186	C11H22O2	000112-37-8	27





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Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
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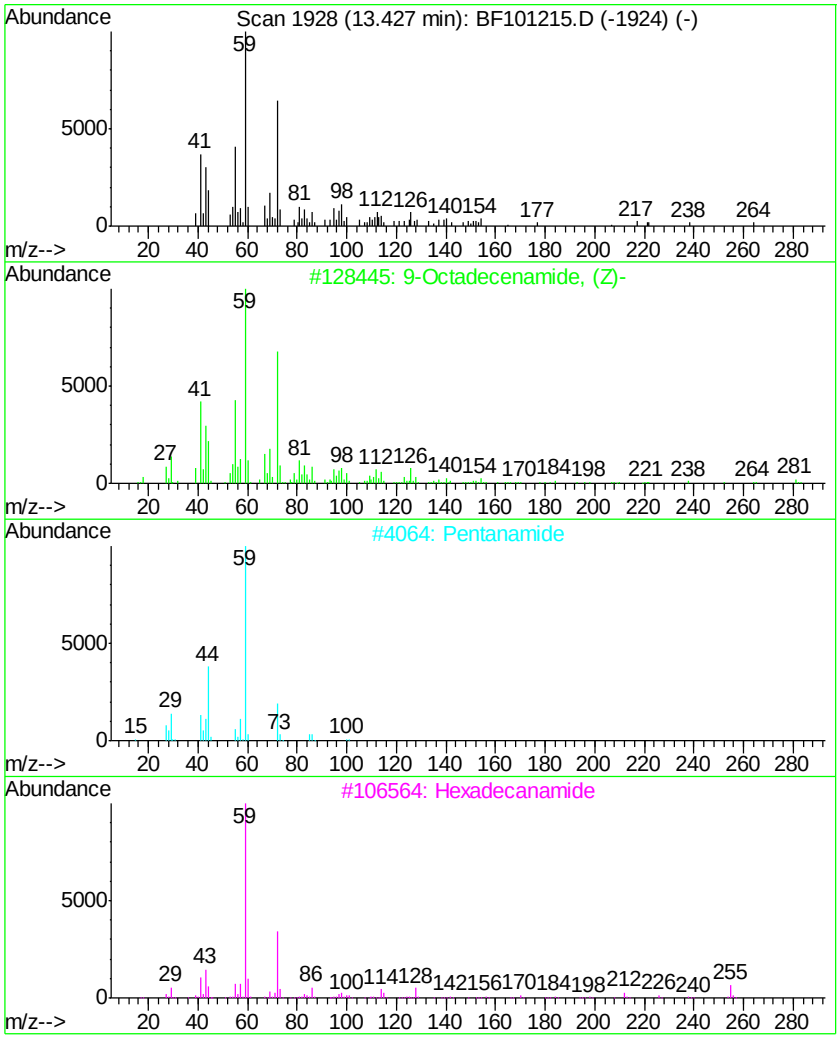
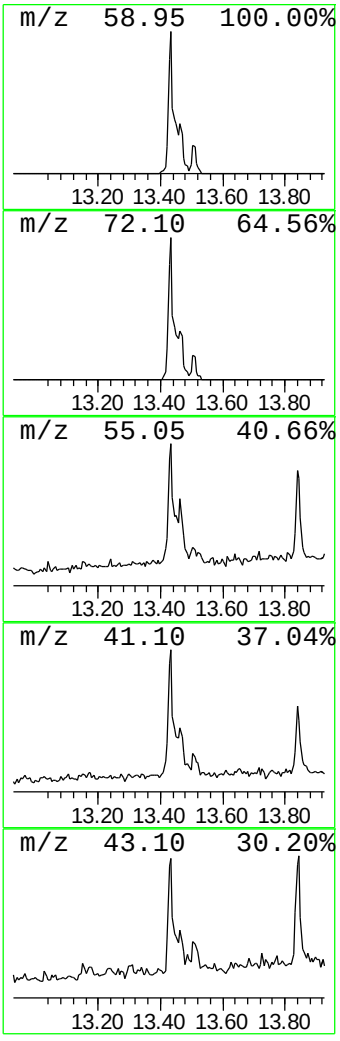
Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	10.26 ng	171819	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2	Pentanamide	101	C5H11NO	000626-97-1	59
3	Hexadecanamide	255	C16H33NO	000629-54-9	53
4	Methyl 17-methoxy-10-methoxycarb...	386	C22H42O5	1000110-20-7	43
5	Silane, hexyl-	116	C6H16Si	001072-14-6	43





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Misc :
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ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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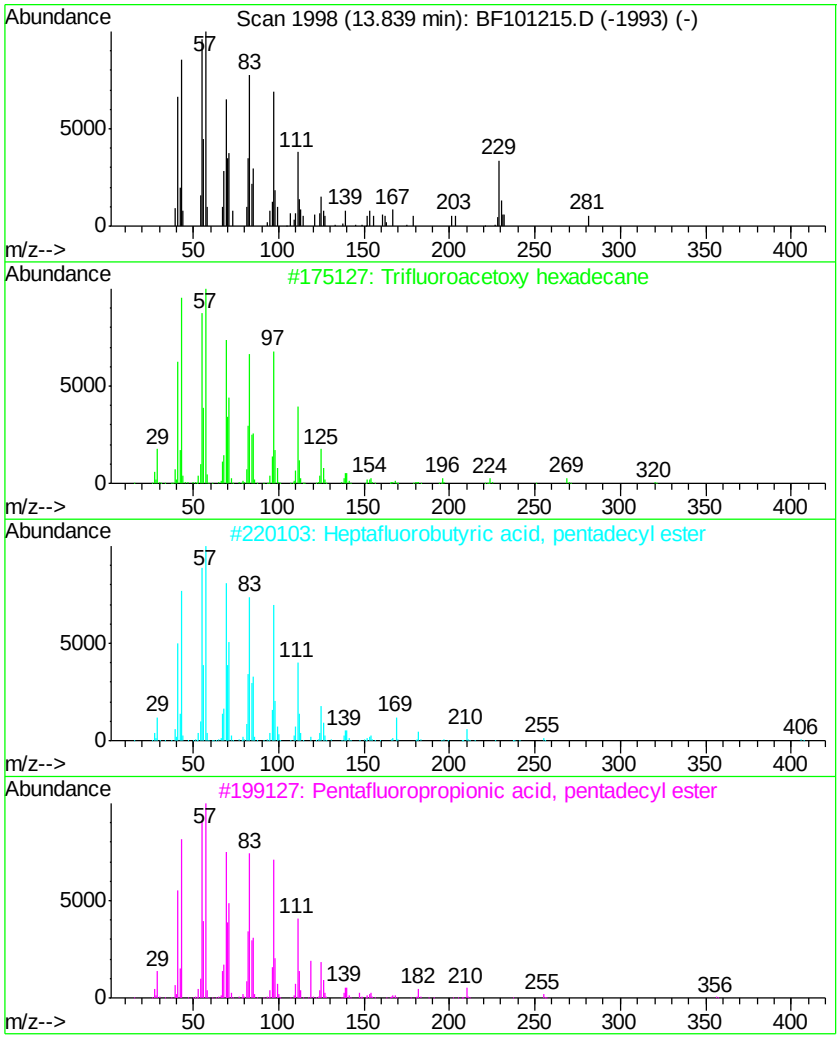
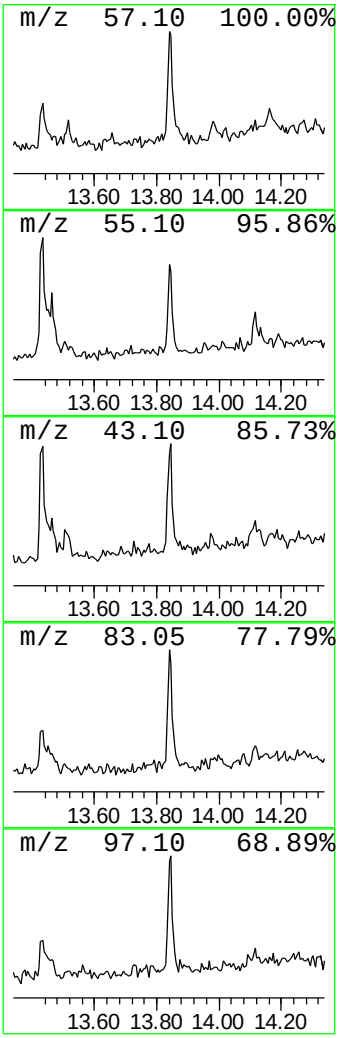
Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	4.55 ng	76219	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	1-Docosene	308	C22H44	001599-67-3	93
5	1-Octadecanol	270	C18H38O	000112-92-5	93





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

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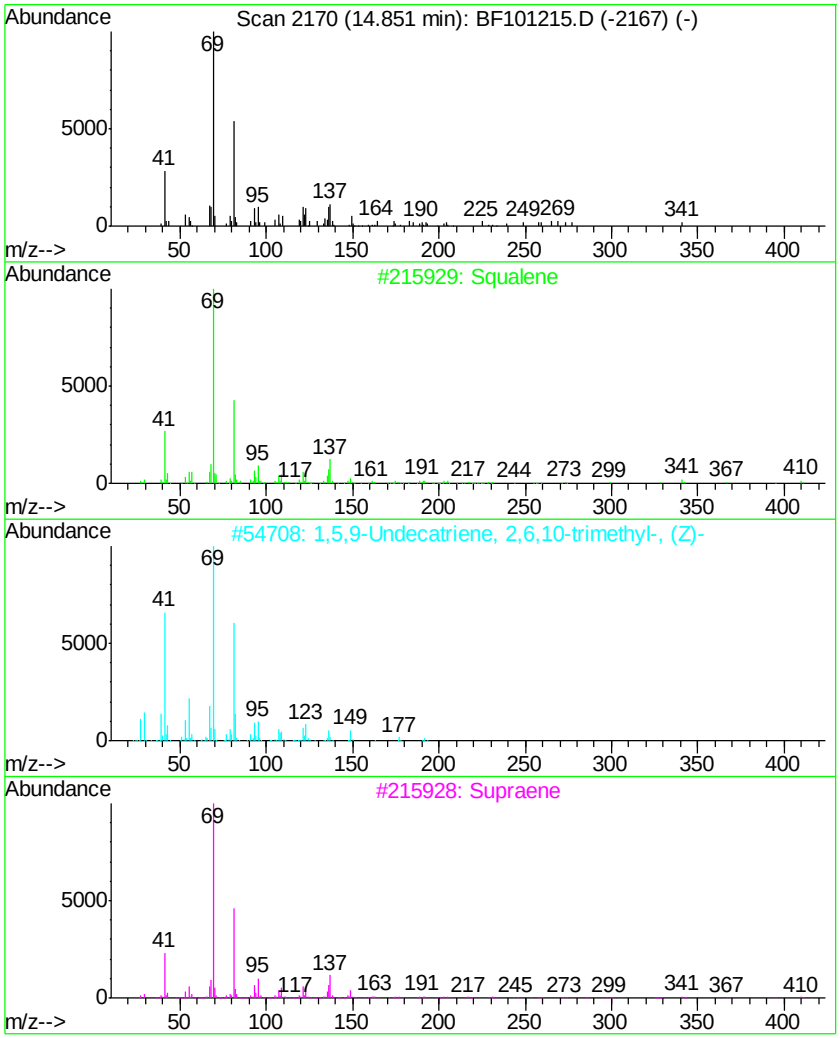
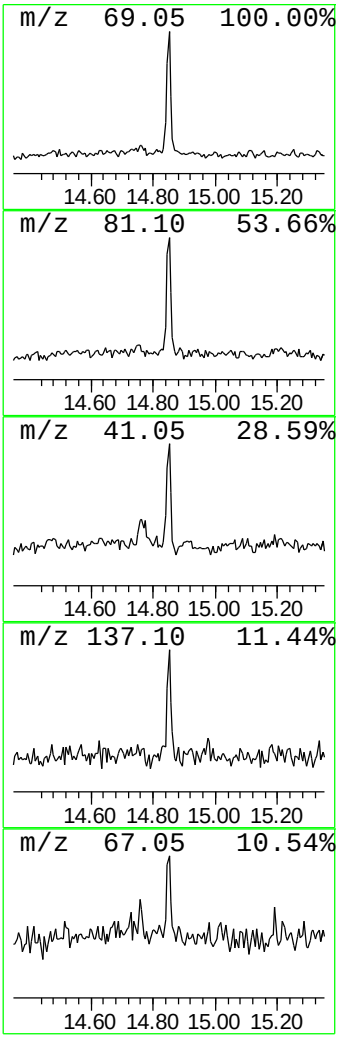
Peak Number 10 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	7.52 ng	78291	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
3	Supraene	410	C30H50	007683-64-9	87
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
5	trans-Farnesol	222	C15H26O	000106-28-5	64





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Data File : BF101215.D
Acq On : 7 Dec 2017 19:46
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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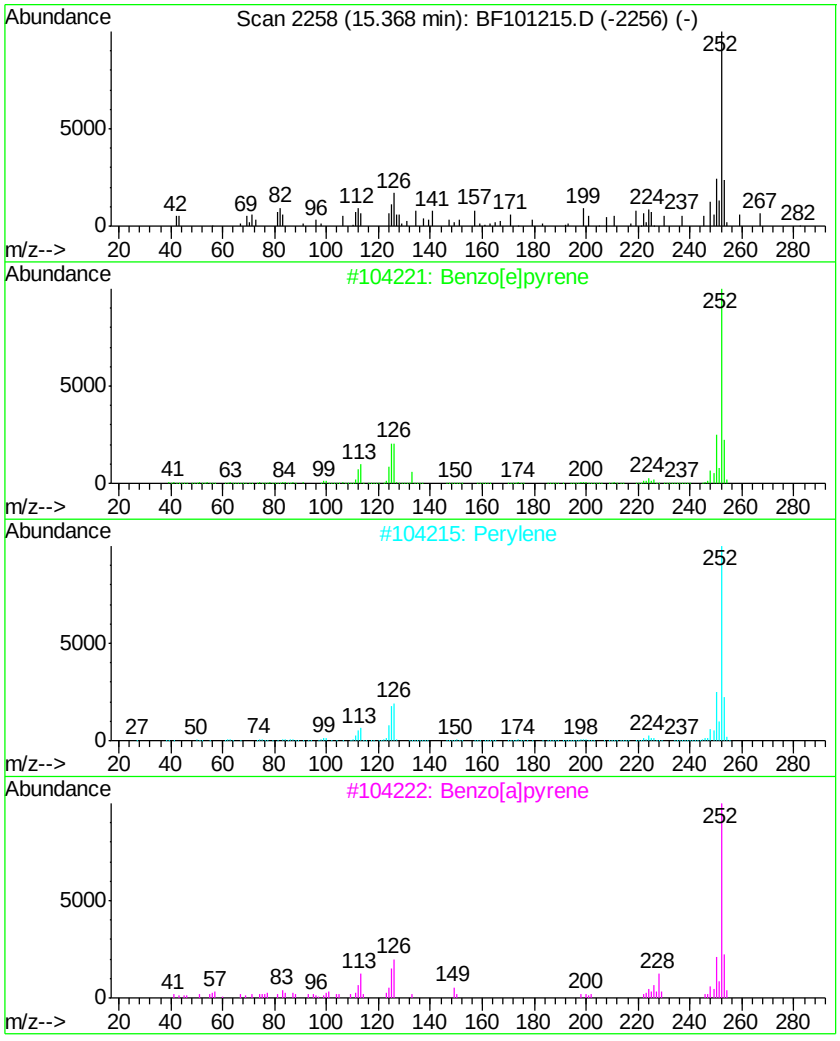
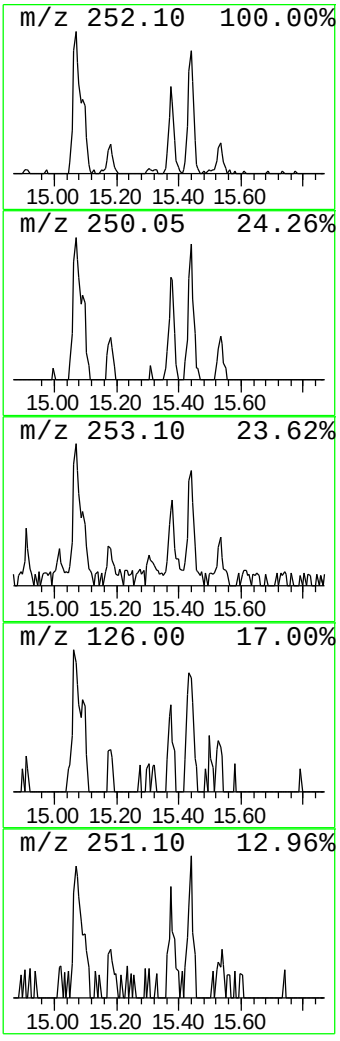
Peak Number 11 Benzo[e]pyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	3.42 ng	35638	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	70
2	Perylene	252	C20H12	000198-55-0	70
3	Benzo[a]pyrene	252	C20H12	000050-32-8	62
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	58
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF120717\
Data File : BF101215.D
Acq On : 7 Dec 2017 19:46
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.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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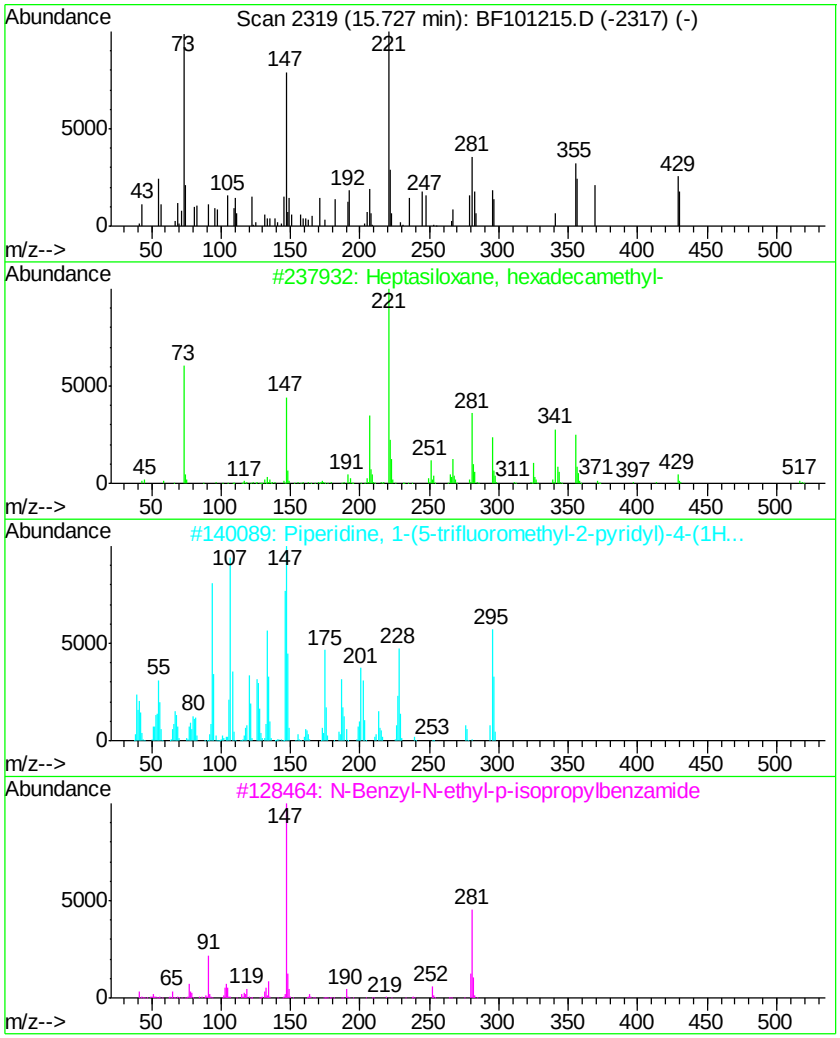
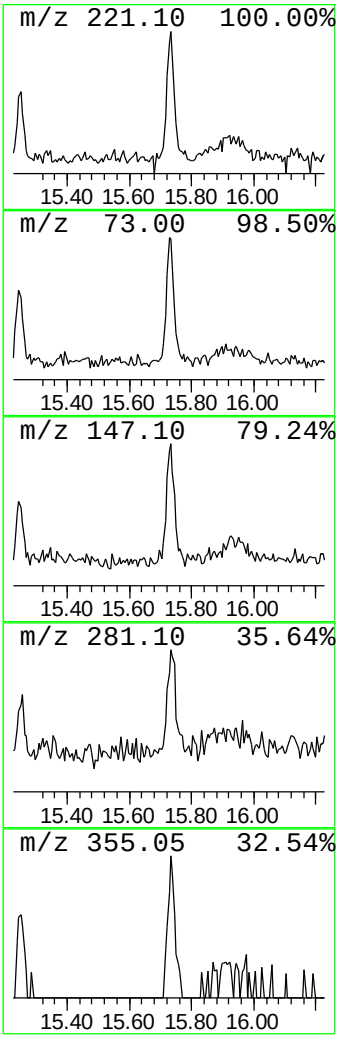
Peak Number 12 unknown15.75 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	4.60 ng	47821	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	40
2	Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	25
3	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	14
4	2-((E)-([3-(2-Dimethylanilino)-1...	356	C23H20N2O2	073428-83-8	14
5	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	12





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Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Integration Parameters: LSCINT.P

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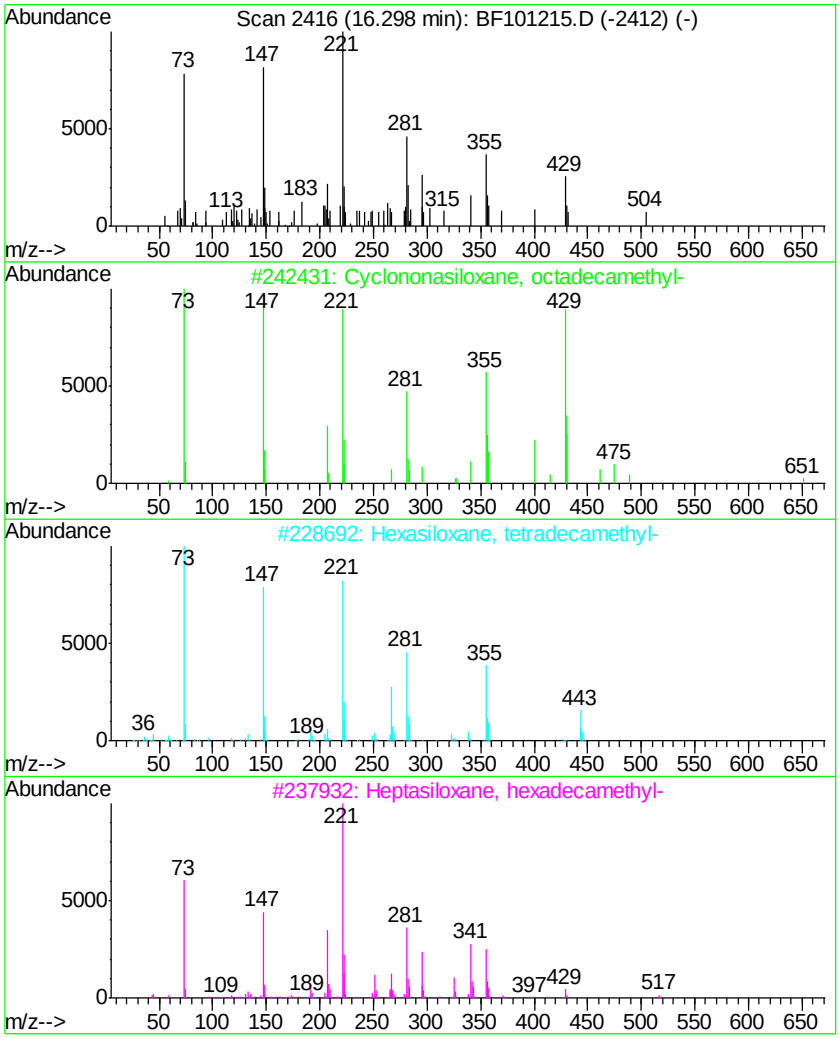
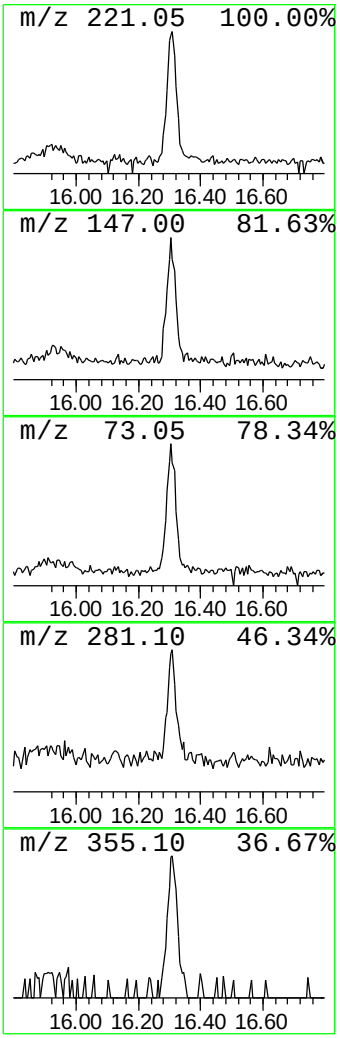
Peak Number 13 Cyclononasiloxane, octadeca... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.30	7.49 ng	77952	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	59
3	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	38
4	Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	35
5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	32





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Data File : BF101215.D
Acq On : 7 Dec 2017 19:46
Operator : SJ/JU
Sample : I6717-03
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB-3(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF113017.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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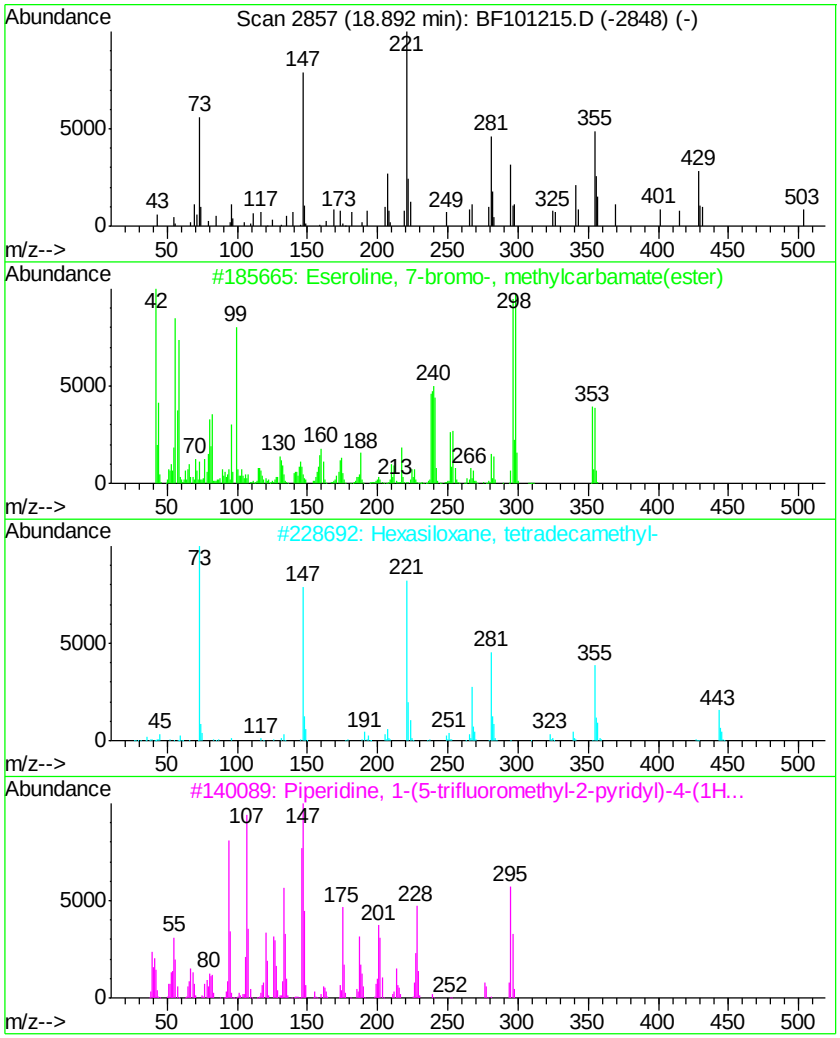
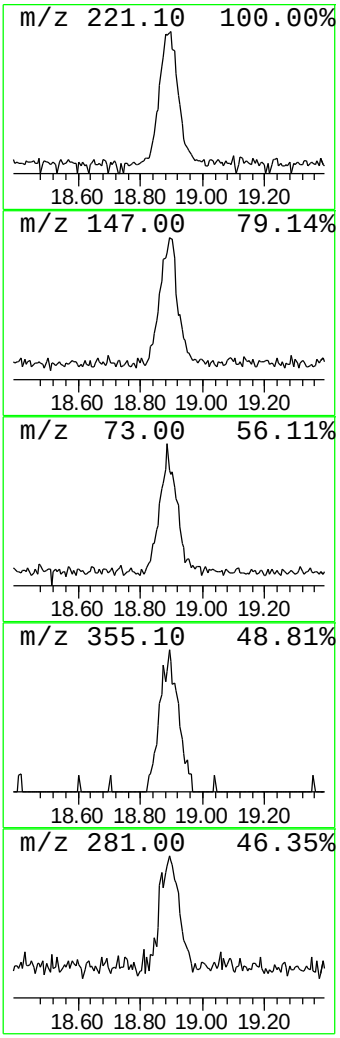
Peak Number 15 Eseroline, 7-bromo-, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.89	13.07 ng	135968	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eseroline, 7-bromo-, methylcarba...	353	C15H20BrN3O2	114546-23-5	92
2	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	59
3	Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	56
4	Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	43
5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF120717\
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Operator : SJ/JU
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Instrument : BNA_F
ClientSampleId : PB-3(0-10)

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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...	5.07	5.7	ng	73071	1	6.84	256690	20.0
unknown6.62	6.62	83.2	ng	1067360	1	6.84	256690	20.0
Tetracosane	10.77	2.0	ng	27960	4	11.37	273143	20.0
unknown11.89	11.89	2.9	ng	39988	4	11.37	273143	20.0
9-Octadecenamide,...	13.43	10.3	ng	171819	5	14.02	334950	20.0
Trifluoroacetoxy ...	13.84	4.5	ng	76219	5	14.02	334950	20.0
Squalene	14.85	7.5	ng	78291	6	15.50	208135	20.0
Benzo[e]pyrene	15.37	3.4	ng	35638	6	15.50	208135	20.0
unknown15.75	15.73	4.6	ng	47821	6	15.50	208135	20.0
Cyclononasiloxane...	16.30	7.5	ng	77952	6	15.50	208135	20.0
Eseroline, 7-brom...	18.89	13.1	ng	135968	6	15.50	208135	20.0