LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

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-BF110818.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	2.252	24	28	37	rVB	92018	130417	5.54%	0.599%
2	5.187	523	527	538	rBV	50456	79310	3.37%	0.364%
3	5.569	587	592	613	rBV	1753968	1883781	79.99%	8.651%
4	6.575	758	763	780	rBV	1838029	2096762	89.03%	9.629%
5	6.716	783	787	790	rBV	2229415	1995894	84.75%	9.166%
6	6.945	822	826	832	rBV	466836	442630	18.80%	2.033%
7	7.098	848	852	867	rBV	1773213	1575661	66.91%	7.236%
8	7.510	918	922	945	rBV	1296629	1285008	54.57%	5.901%
9	8.222	1040	1043	1060	rBV	547529	615495	26.14%	2.827%
10	9.298	1222	1226	1229	rBV	2742857	2355000	100.00%	10.815%
11	9.692	1289	1293	1300	rVB	207977	195865	8.32%	0.900%
12	9.986	1337	1343	1346	rBV	660000	656034	27.86%	3.013%
13	10.016	1346	1348	1354	rVB	55659	50582	2.15%	0.232%
14	10.539	1433	1437	1443	rVB	37799	39828	1.69%	0.183%
15	10.780	1473	1478	1488	rBV	1195510	1265063	53.72%	5.810%
16	11.480	1593	1597	1599	rBV	661394	603188	25.61%	2.770%
17	11.504	1599	1601	1605	rVV	355059	300063	12.74%	1.378%
18	11.557	1605	1610	1615	rVB	75444	74830	3.18%	0.344%
19	11.980	1679	1682	1685	rBV	144741	131826	5.60%	0.605%
20	12.010	1685	1687	1693	rVB	41743	42591	1.81%	0.196%
21	12.098	1698	1702	1704	rBV2	65639	68577	2.91%	0.315%
22	12.698	1800	1804	1809	rBV	554938	493637	20.96%	2.267%
23	12.768	1812	1816	1818	rBV2	27757	29786	1.26%	0.137%
24	12.851	1826	1830	1836	rBV2	17708	27874	1.18%	0.128%
25	12.910	1836	1840	1841	rBV	86646	92116	3.91%	0.423%
26	12.927	1841	1843	1848	rVB	458658	393268	16.70%	1.806%
27	13.063	1861	1866	1869	rBV	1892746	1746194	74.15%	8.019%
28	13.257	1891	1899	1906	rBV	74241	123495	5.24%	0.567%
29	13.321	1907	1910	1913	rVV	61900	53291	2.26%	0.245%
30	13.880	2002	2005	2007	rBV	37692	35997	1.53%	0.165%
31	13.933	2011	2014	2020	rVV2	237209	281834	11.97%	1.294%
32	14.127	2042	2047	2050	rBV2	569707	691781	29.37%	3.177%
33	14.157	2050	2052	2059	rVB	181442	168441	7.15%	0.774%
34	14.233	2063	2065	2067	rBV	41148	46122	1.96%	0.212%

LSC Area Percent Report

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Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

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-BF110818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.557	2117	2120	2125	rBV3	42503	77387	3.29%	0.355%
36	14.868	2171	2173	2178	rVB	55771	63498	2.70%	0.292%
37	14.951	2185	2187	2191	rBV3	27036	32454	1.38%	0.149%
38	15.204	2226	2230	2240	rBV2	193079	430325	18.27%	1.976%
39	15.315	2247	2249	2254	rVB	46019	48216	2.05%	0.221%
40	15.457	2270	2273	2275	rBV4	19471	28884	1.23%	0.133%
41	15.521	2281	2284	2288	rBV	93832	104314	4.43%	0.479%
42	15.592	2292	2296	2299	rBV	150902	211667	8.99%	0.972%
43	15.657	2303	2307	2311	rBV	284828	351748	14.94%	1.615%
44	16.068	2373	2377	2382	rVB	53275	83162	3.53%	0.382%
45	16.592	2462	2466	2471	rBV2	31605	55534	2.36%	0.255%
46	17.227	2569	2574	2582	rVB2	64709	145081	6.16%	0.666%
47	17.709	2651	2656	2662	rBV	37252	69898	2.97%	0.321%

Sum of corrected areas: 21774409

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Instrument : BNA_F
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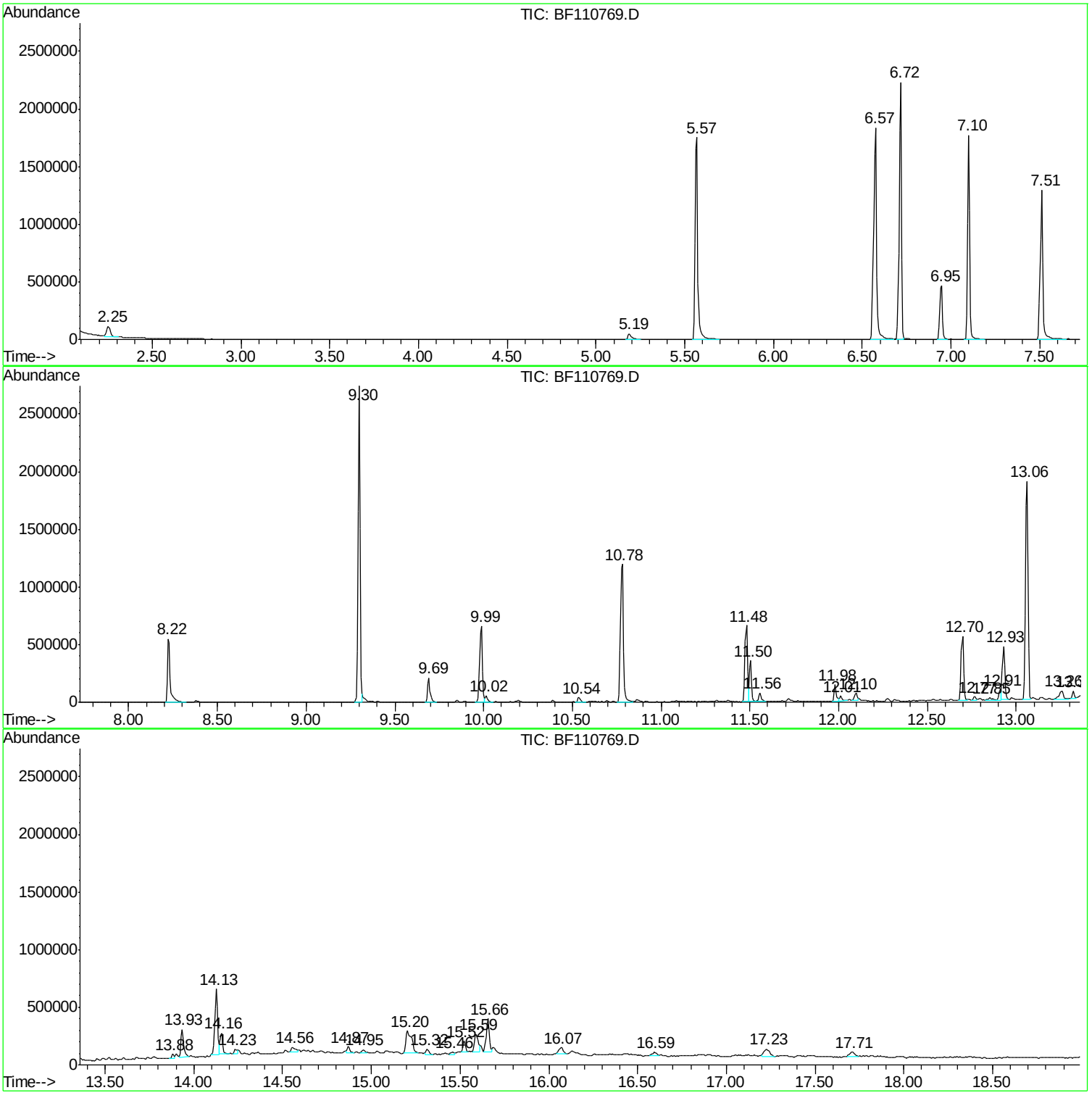
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Operator : JU/SJ
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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

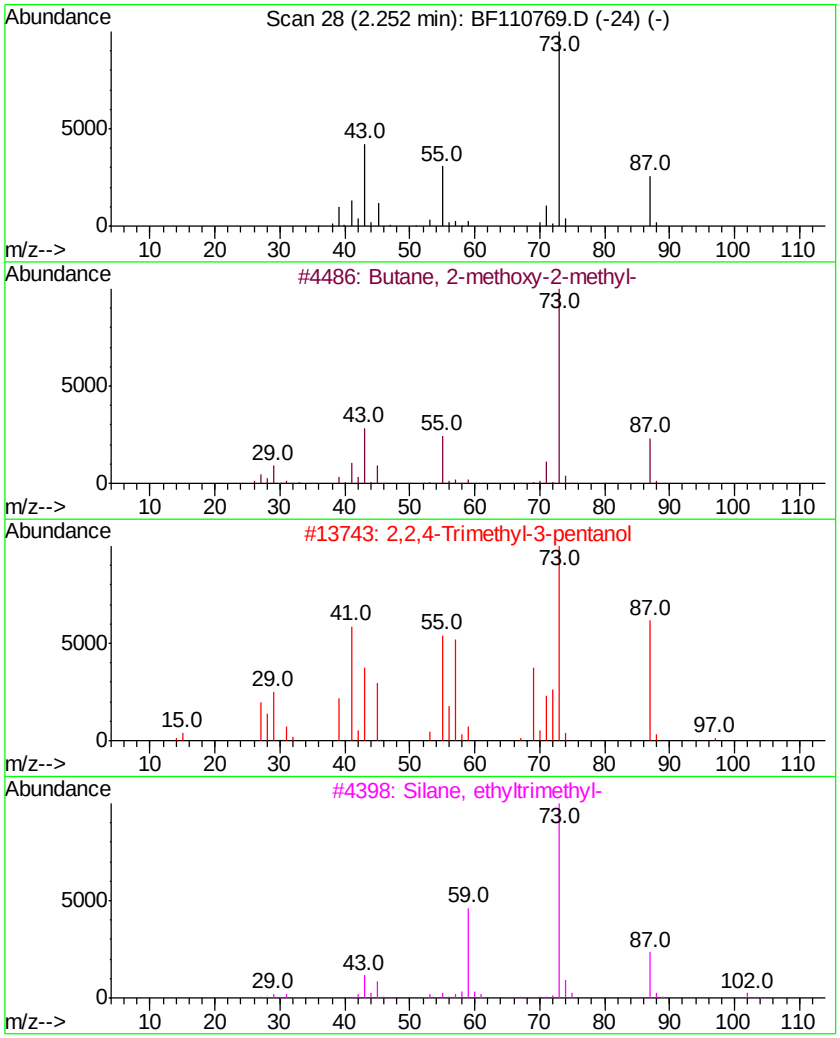
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

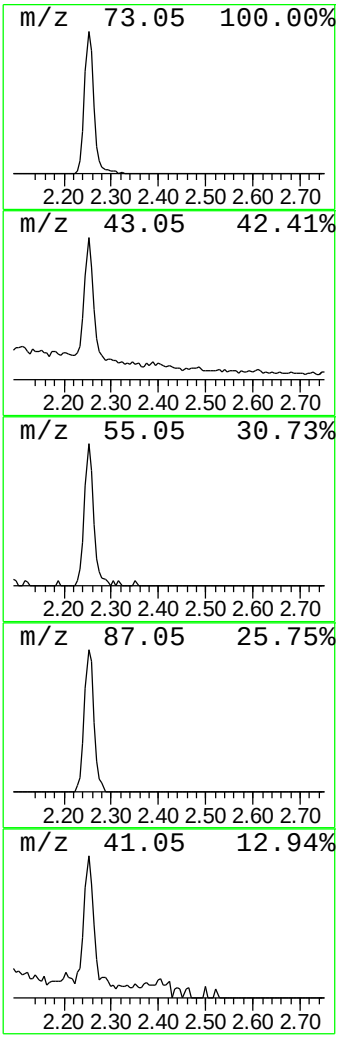
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	5.89 ng	130417	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25





Library Search Compound Report

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Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

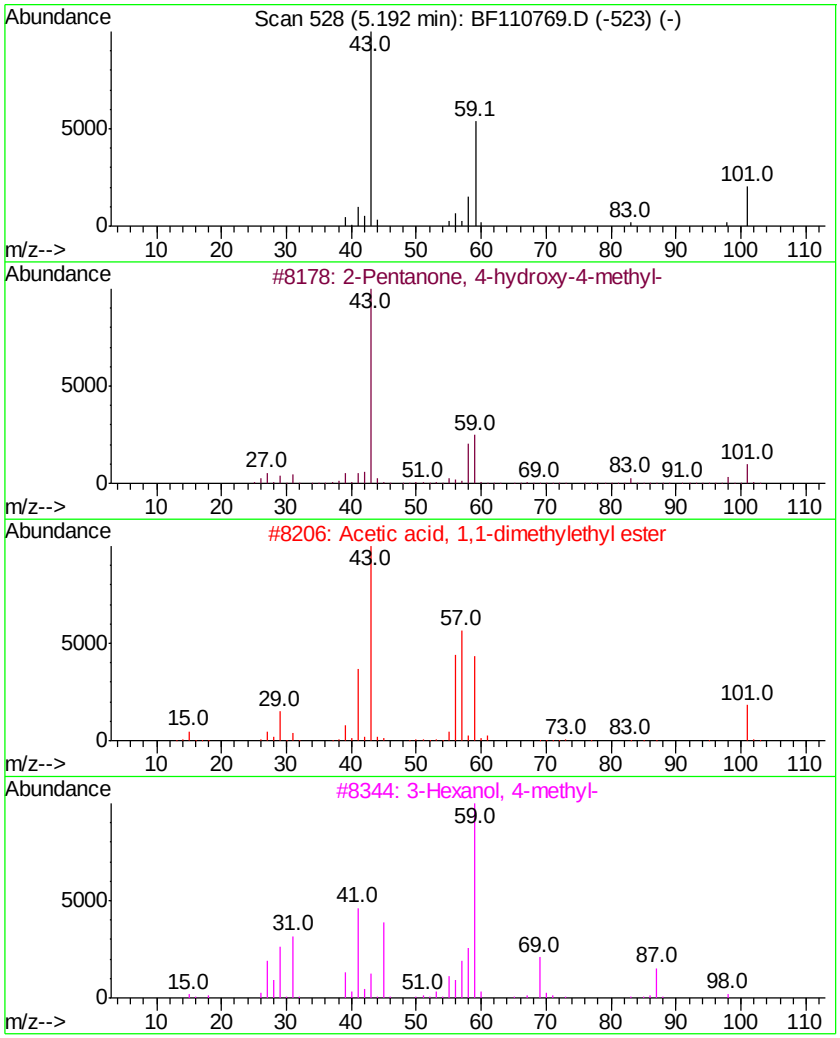
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

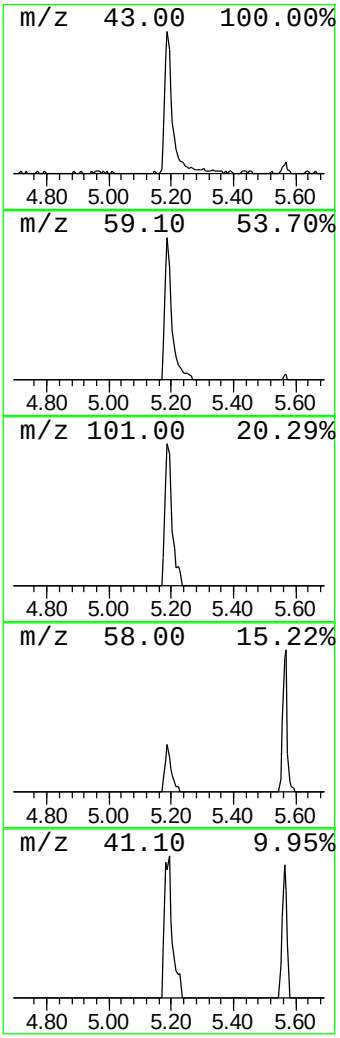
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.58 ng	79310	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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	Acetone	58	C3H6O	000067-64-1	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

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Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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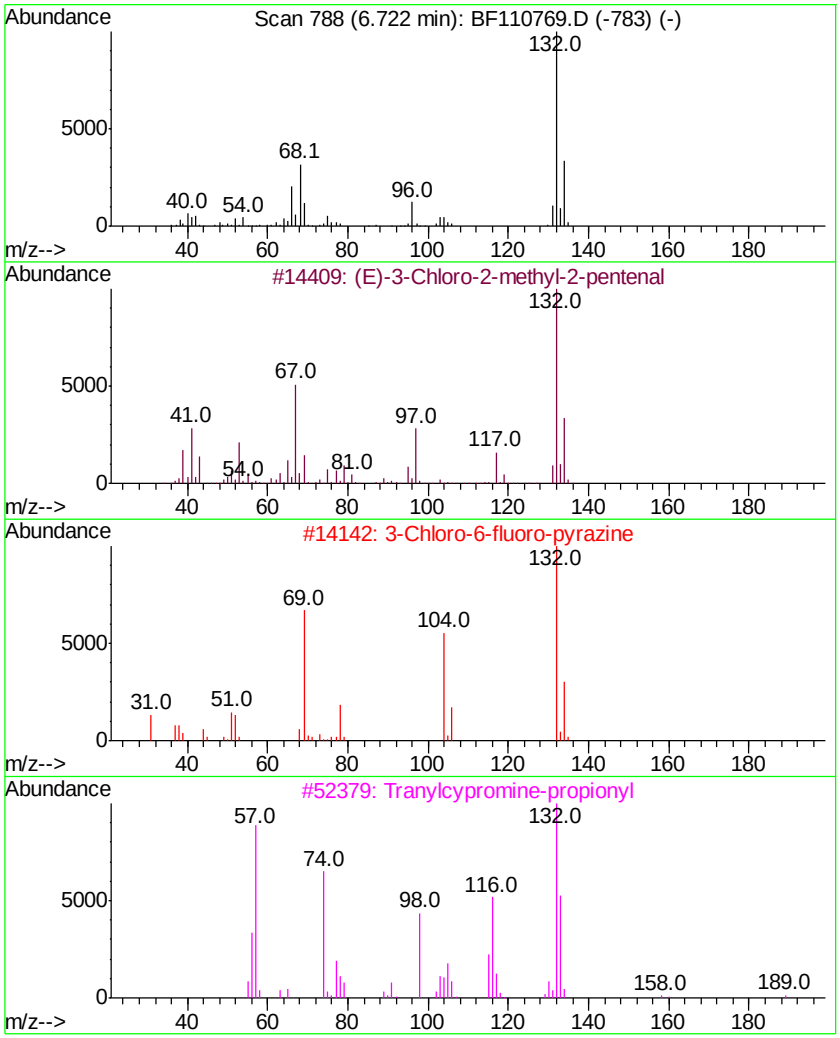
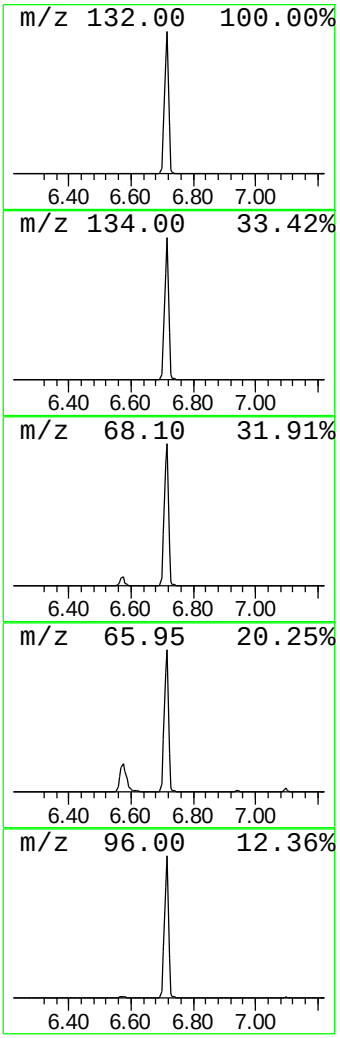
Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	90.18 ng	1995890	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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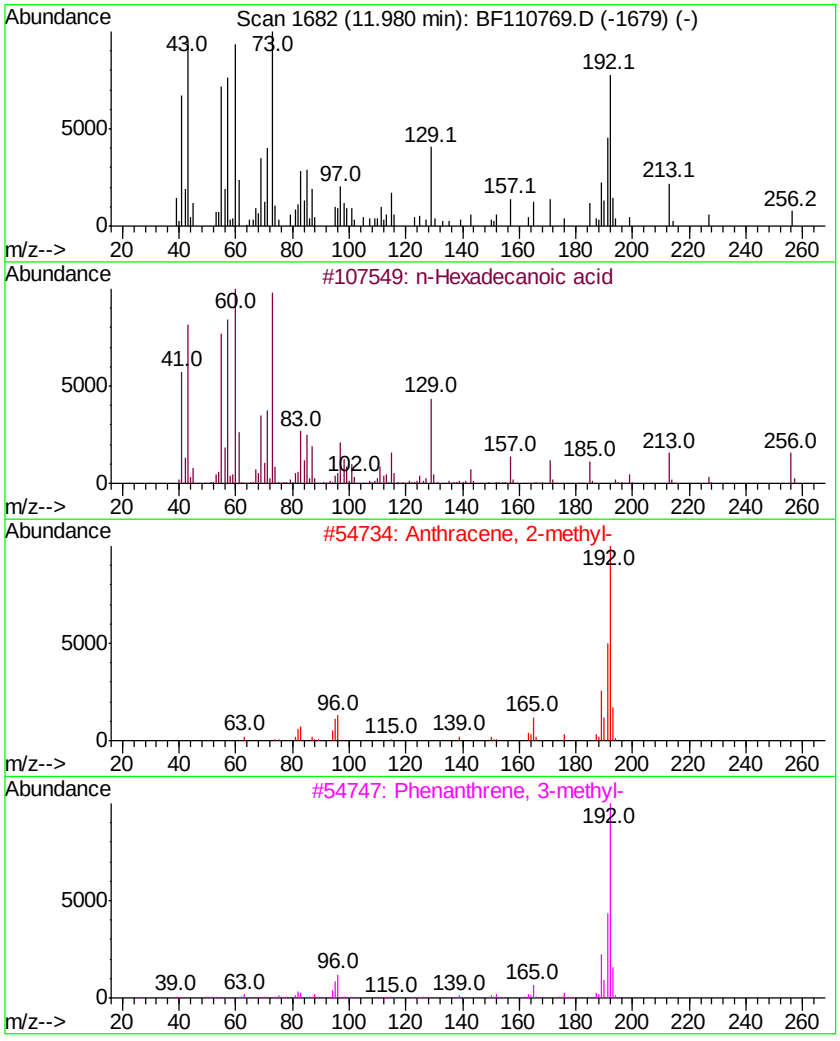
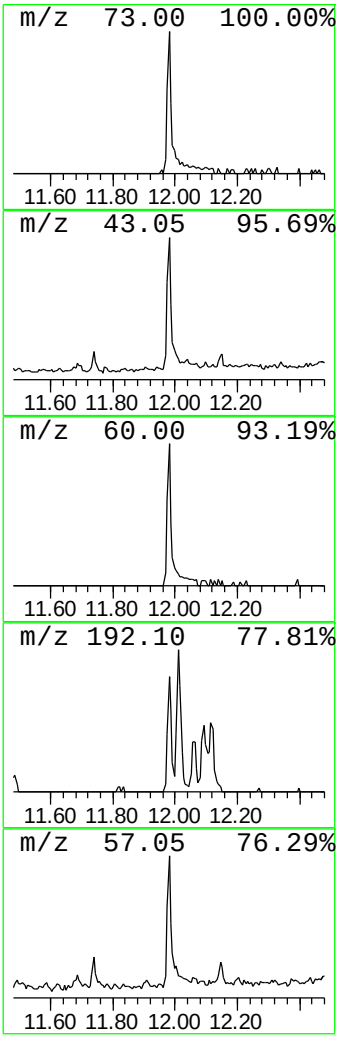
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.98	4.37 ng	131826	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
3	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	62
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	60
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	55





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
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Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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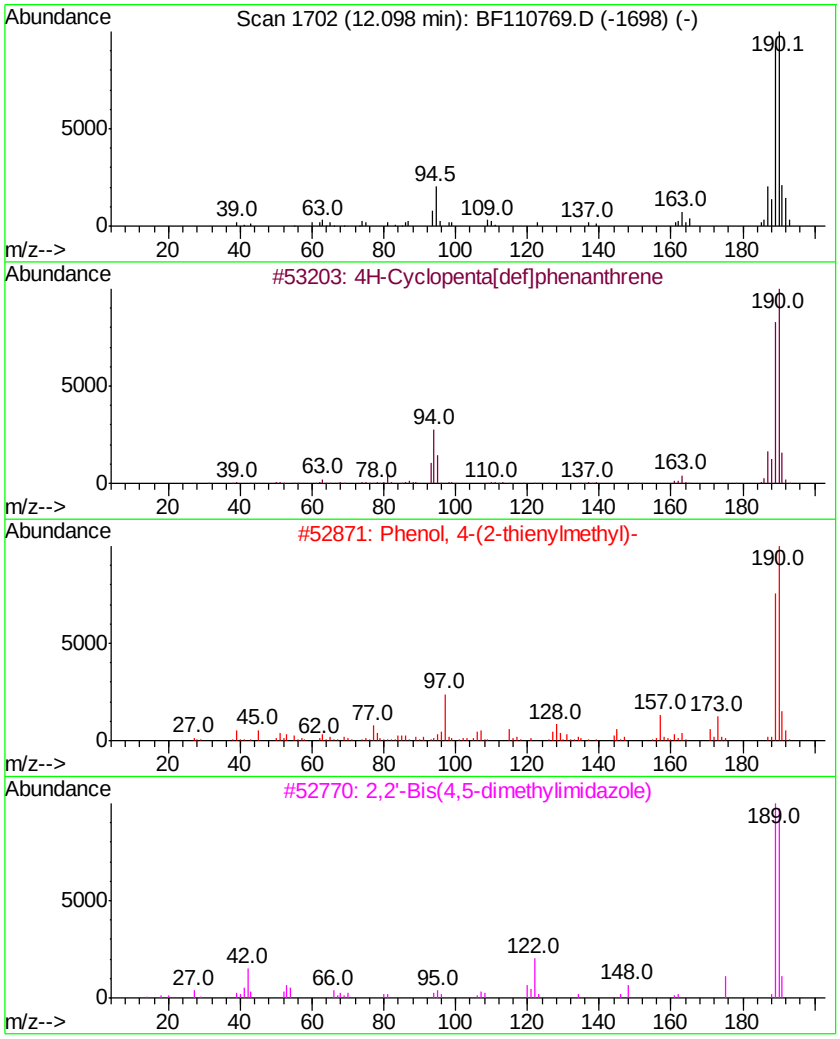
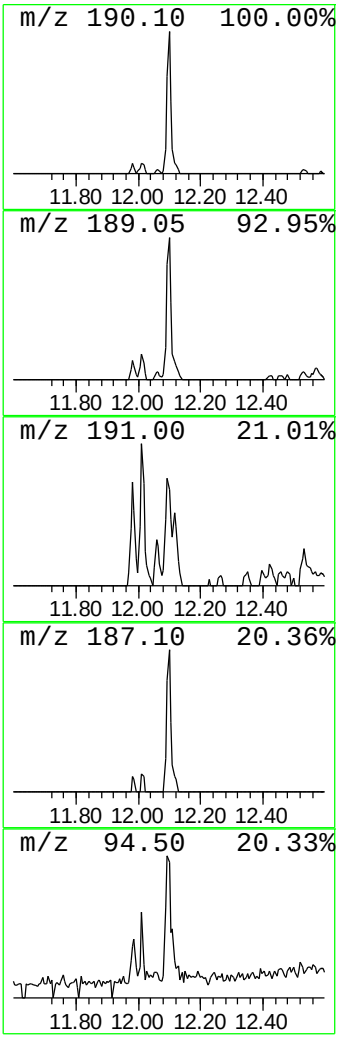
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.10	2.27 ng	68577	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	91
2	Phenol, 4-(2-thienylmethyl)-	190	C11H10OS	091680-55-6	59
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	50
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
5	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	16





Library Search Compound Report

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Data File : BF110769.D
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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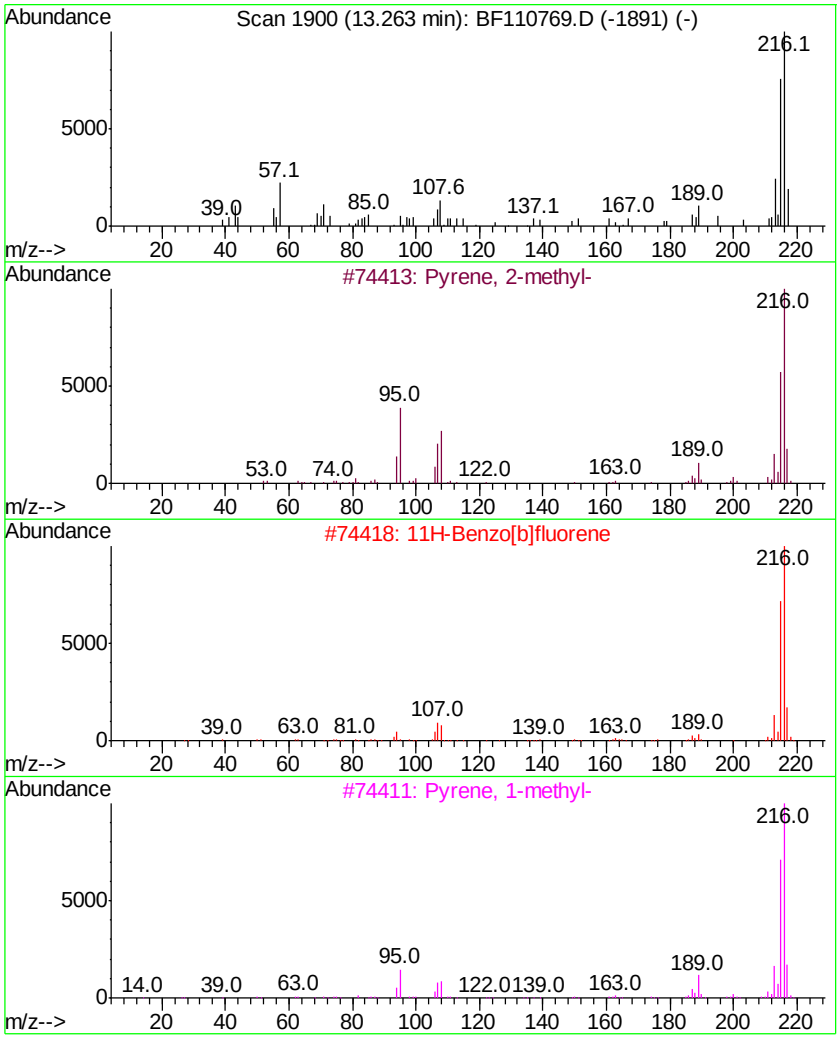
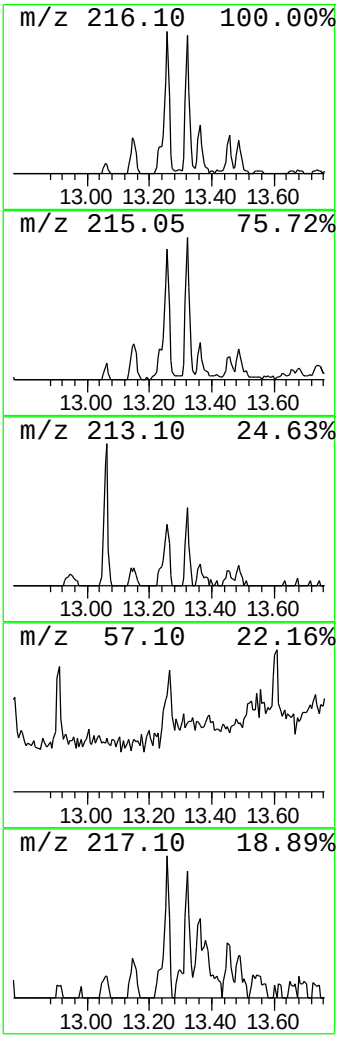
Peak Number 7 Pyrene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	3.57 ng	123495	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	91
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87





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Instrument : BNA_F
ClientSampleId : WALL-A

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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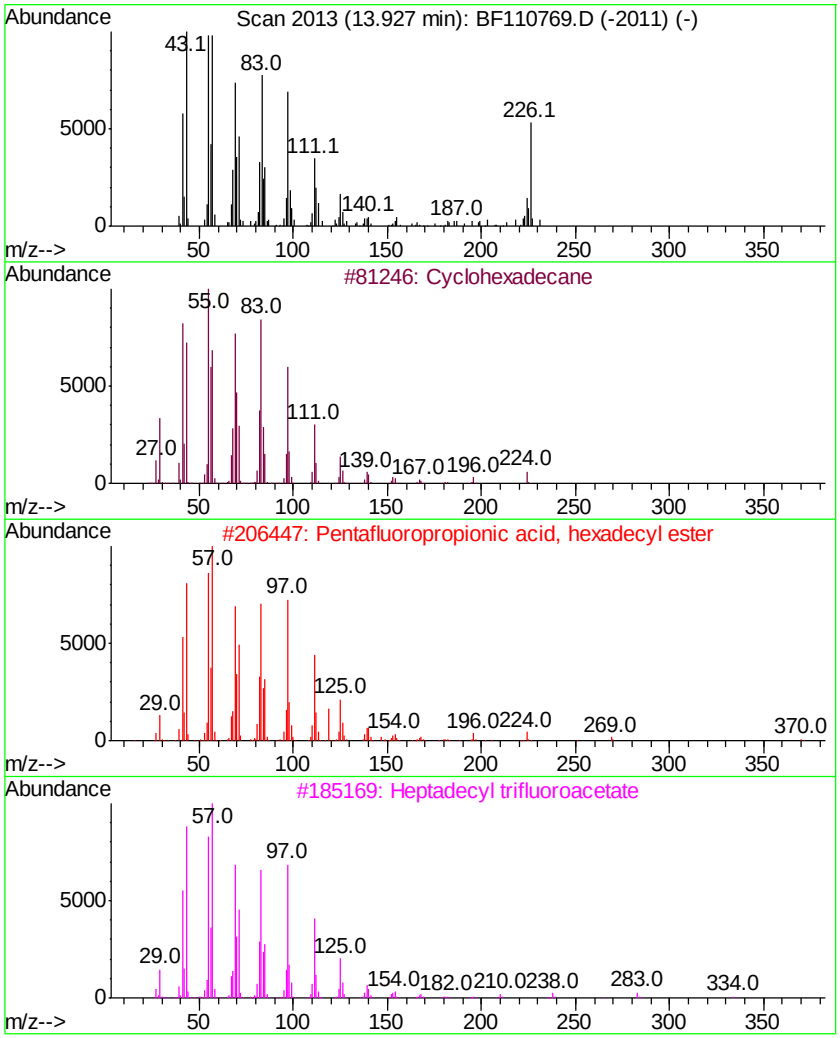
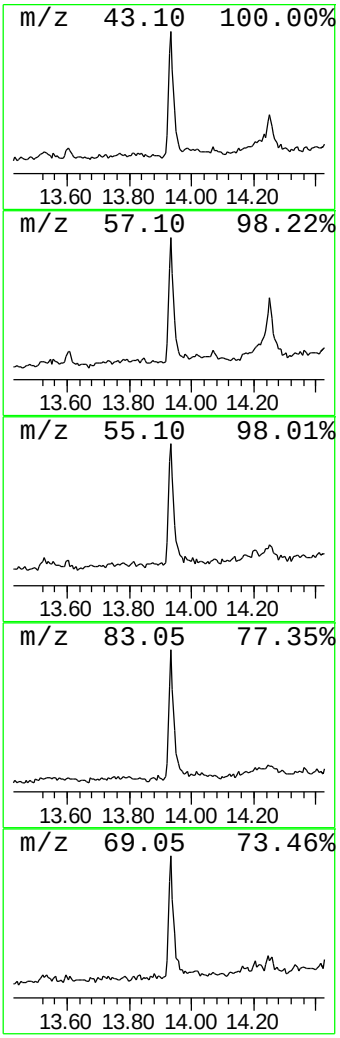
Peak Number 8 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	8.15 ng	281834	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	99
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





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Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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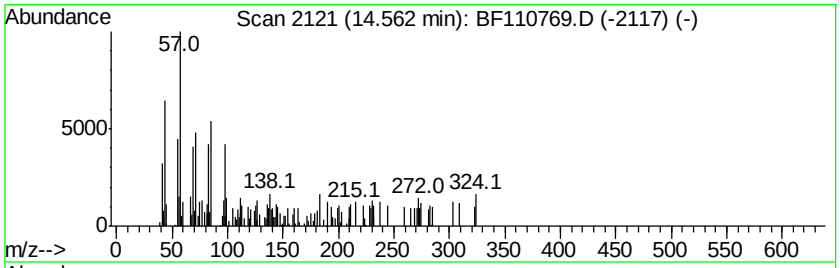
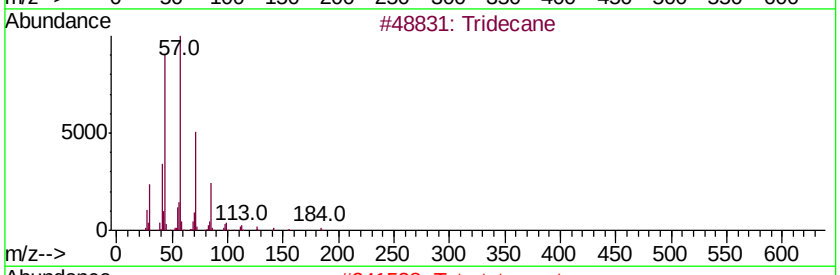
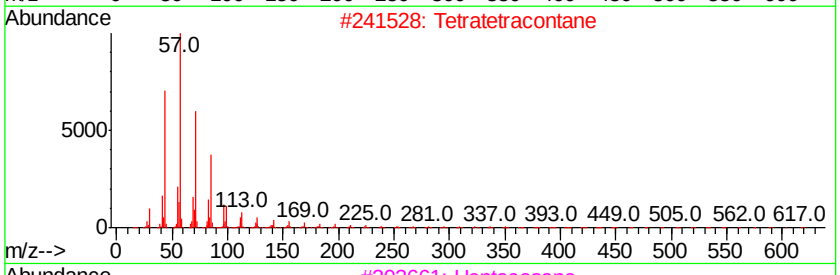
Peak Number 9 Tridecane Concentration Rank 13

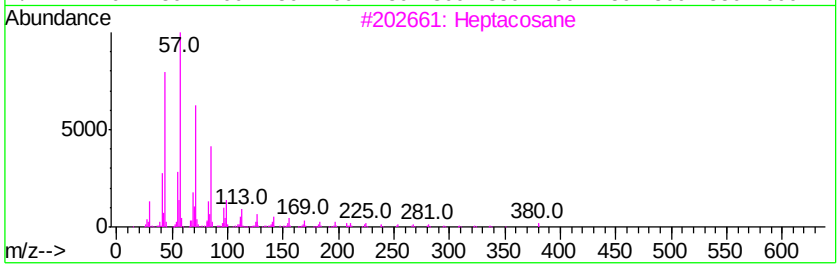
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.24 ng	77387	Chrysene-d12	14.13

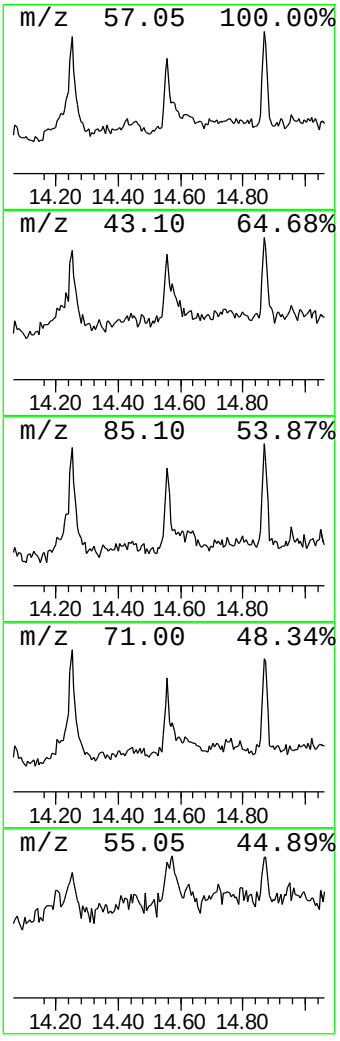
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	49
2	Tetratetracontane	619	C44H90	007098-22-8	49
3	Heptacosane	380	C27H56	000593-49-7	49
4	Heptadecane	240	C17H36	000629-78-7	46
5	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	46











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Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

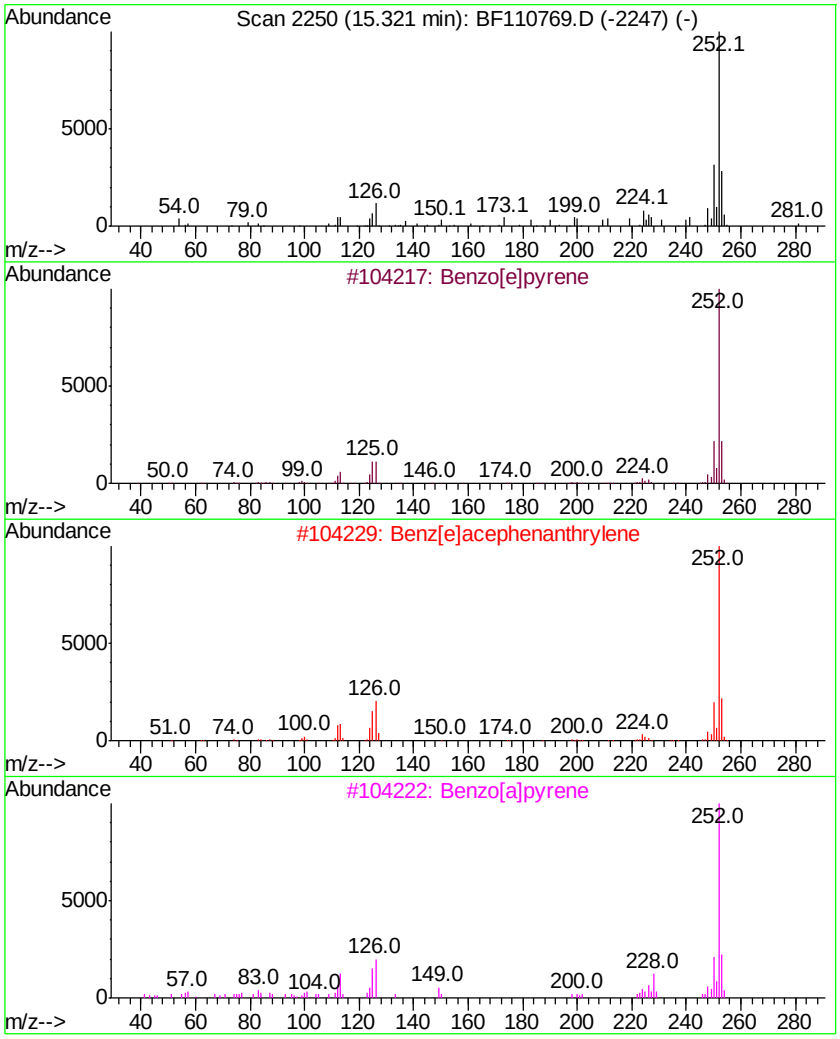
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

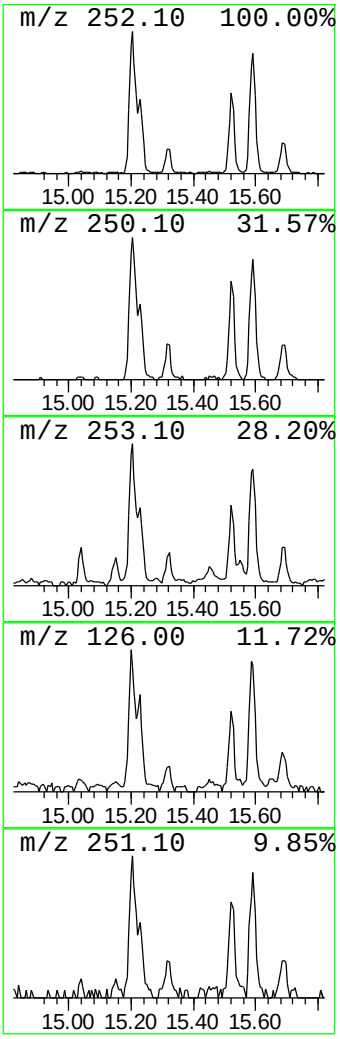
****

Peak Number 10 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	2.74 ng	48216	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	76
3	Benzo[a]pyrene	252	C20H12	000050-32-8	76
4	Perylene	252	C20H12	000198-55-0	70
5	Chromium, (.eta.5-2,4-cyclopenta...	252	C15H20Cr	135162-31-1	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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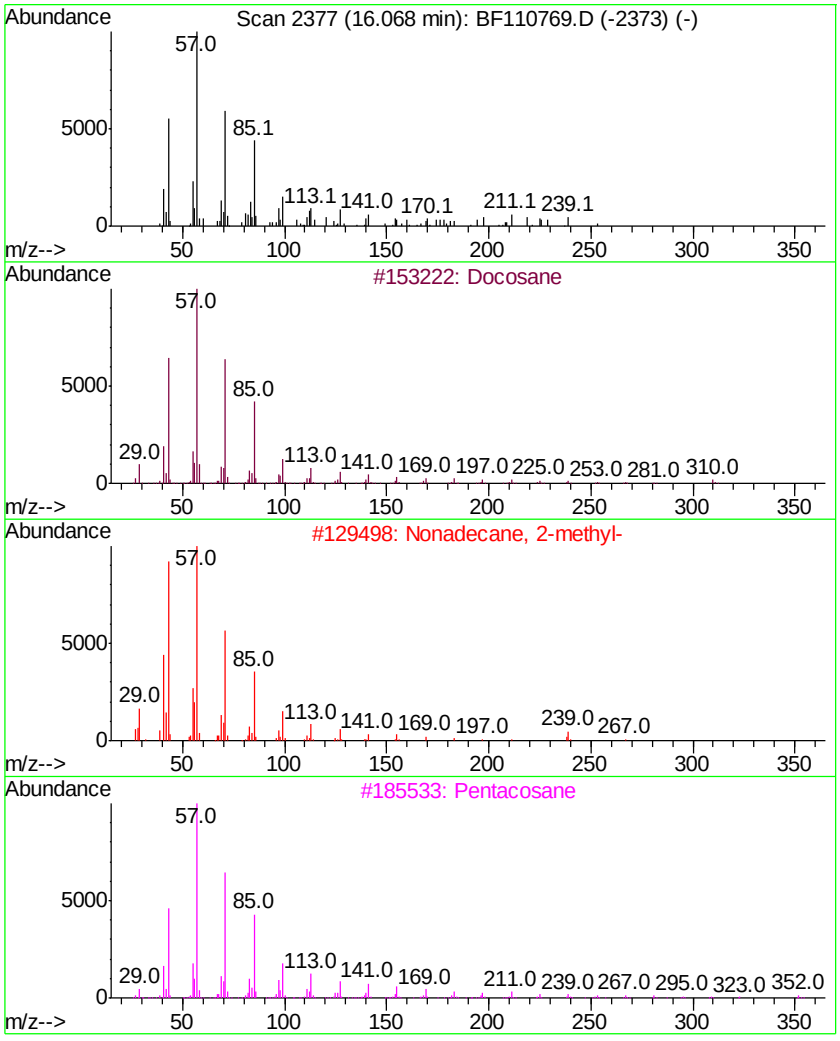
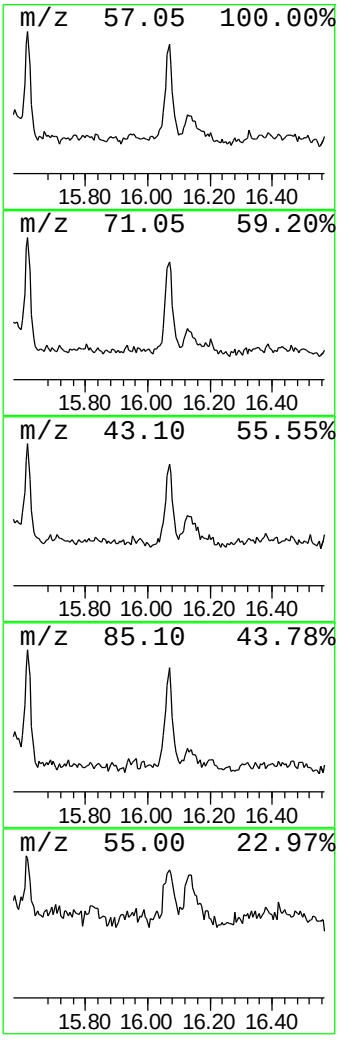
Peak Number 12 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	4.73 ng	83162	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	86
2	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	86
3	Pentacosane	352	C25H52	000629-99-2	83
4	Tetracosane	338	C24H50	000646-31-1	83
5	Hexadecane	226	C16H34	000544-76-3	81





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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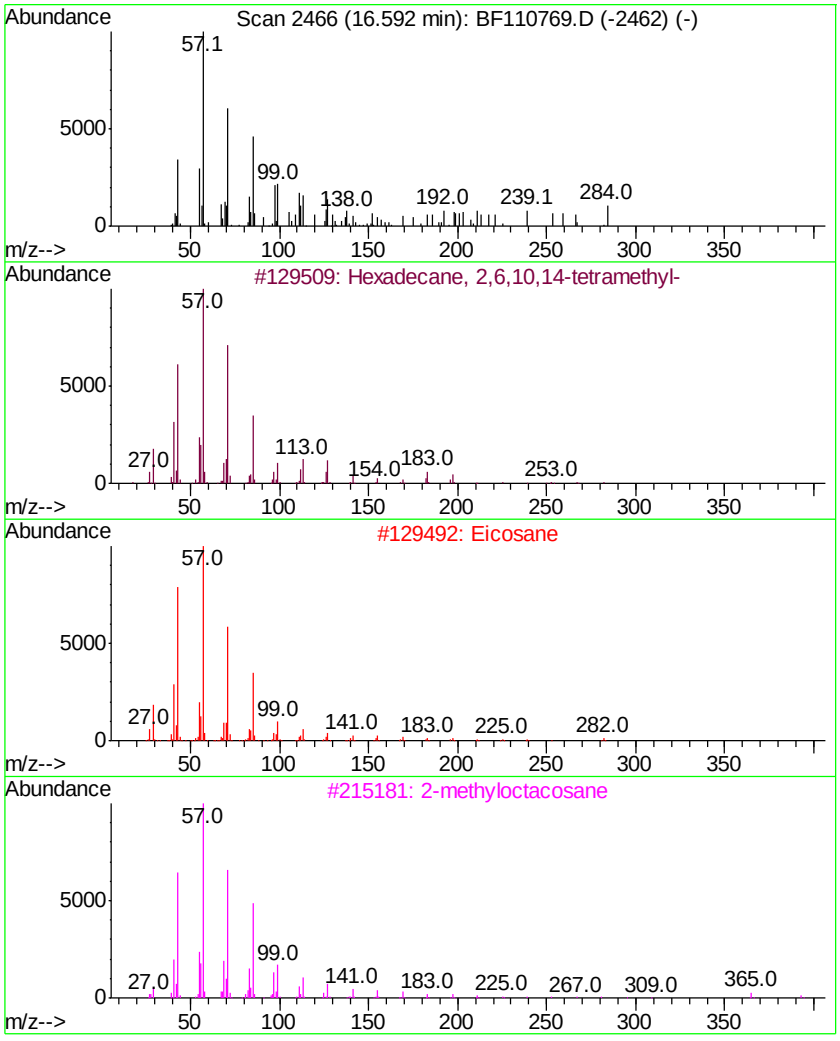
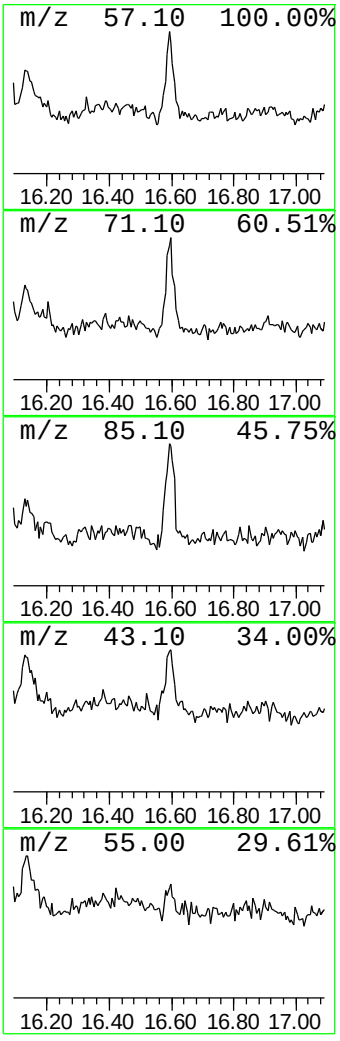
Peak Number 13 Hexadecane, 2,6,10,14-tetra... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.59	3.16 ng	55534	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	64
2	Eicosane	282	C20H42	000112-95-8	64
3	2-methyloctacosane	408	C29H60	1000376-72-8	64
4	Nonacosane	408	C29H60	000630-03-5	59
5	Tetradecane	198	C14H30	000629-59-4	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111418\
Data File : BF110769.D
Acq On : 14 Nov 2018 17:28
Operator : JU/SJ
Sample : J5889-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WALL-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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
Butane, 2-methoxy...	2.25	5.9	ng	130417	1	6.95	442630	20.0
2-Pentanone, 4-hy...	5.19	3.6	ng	79310	1	6.95	442630	20.0
unknown6.72	6.72	90.2	ng	1995890	1	6.95	442630	20.0
n-Hexadecanoic acid	11.98	4.4	ng	131826	4	11.48	603188	20.0
4H-Cyclopenta[def...	12.10	2.3	ng	68577	4	11.48	603188	20.0
Pyrene, 2-methyl-	13.26	3.6	ng	123495	5	14.13	691781	20.0
Cyclohexadecane	13.93	8.2	ng	281834	5	14.13	691781	20.0
Tridecane	14.56	2.2	ng	77387	5	14.13	691781	20.0
Benzo[e]pyrene	15.32	2.7	ng	48216	6	15.66	351748	20.0
Docosane	16.07	4.7	ng	83162	6	15.66	351748	20.0
Hexadecane, 2,6,1...	16.59	3.2	ng	55534	6	15.66	351748	20.0