

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
 Data File : BF118700.D
 Acq On : 24 Jan 2020 22:03
 Operator : CG/JU
 Sample : L1242-11
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20200064-AMENDED-COMP-2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF012020.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	2.140	3	9	21	rVB	998641	1363519	15.23%	2.791%
2	5.104	501	513	516	rBV	4896653	8954037	100.00%	18.326%
3	5.481	573	577	581	rVB	1209686	1002426	11.20%	2.052%
4	6.392	729	732	736	rBV	196027	175537	1.96%	0.359%
5	6.486	742	748	756	rBV2	2593896	2923971	32.66%	5.984%
6	6.557	756	760	762	rBV	209668	179937	2.01%	0.368%
7	6.692	780	783	788	rVB	999953	765305	8.55%	1.566%
8	6.863	808	812	816	rBV	1791743	1453086	16.23%	2.974%
9	6.928	820	823	826	rVV	413933	361486	4.04%	0.740%
10	7.022	835	839	842	rBV	4701818	3980699	44.46%	8.147%
11	7.186	863	867	870	rBV	135473	112660	1.26%	0.231%
12	7.422	899	907	910	rBV	3156947	2961343	33.07%	6.061%
13	7.575	929	933	936	rVB	971784	771671	8.62%	1.579%
14	7.633	940	943	946	rVV	117484	97209	1.09%	0.199%
15	8.145	1026	1030	1033	rBV	2273298	1836598	20.51%	3.759%
16	9.222	1208	1213	1216	rBV	5408919	4834437	53.99%	9.894%
17	9.610	1275	1279	1283	rVB	1011063	817323	9.13%	1.673%
18	9.898	1324	1328	1332	rVV	2388687	2050996	22.91%	4.198%
19	10.680	1458	1461	1467	rBV	662037	580420	6.48%	1.188%
20	10.804	1478	1482	1490	rVB2	292141	331206	3.70%	0.678%
21	10.992	1511	1514	1517	rBV3	71903	94921	1.06%	0.194%
22	11.045	1520	1523	1527	rVB3	89866	94002	1.05%	0.192%
23	11.239	1552	1556	1562	rBV3	218153	290430	3.24%	0.594%
24	11.380	1576	1580	1583	rBV	2301238	1980743	22.12%	4.054%
25	11.451	1588	1592	1596	rVB2	106393	124828	1.39%	0.255%
26	11.604	1615	1618	1622	rBV	92518	91635	1.02%	0.188%
27	11.904	1667	1669	1674	rBV2	132157	135085	1.51%	0.276%
28	11.998	1682	1685	1691	rVB2	66869	92177	1.03%	0.189%
29	12.163	1711	1713	1717	rVB2	116341	101849	1.14%	0.208%
30	12.592	1783	1786	1789	rVB	282956	230637	2.58%	0.472%
31	12.821	1819	1825	1827	rBV	247781	276478	3.09%	0.566%
32	12.962	1845	1849	1858	rVB	4915820	4240124	47.35%	8.678%
33	13.210	1887	1891	1894	rVB2	74523	95902	1.07%	0.196%
34	13.857	1997	2001	2009	rBV	405984	472679	5.28%	0.967%

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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-BF012020.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.015	2022	2028	2031	rBV	1647225	1716886	19.17%	3.514%
36	14.039	2031	2032	2038	rVB	181679	131308	1.47%	0.269%
37	14.180	2054	2056	2061	rVB2	98643	95171	1.06%	0.195%
38	14.486	2105	2108	2112	rVB2	150598	145289	1.62%	0.297%
39	14.792	2157	2160	2165	rBV	142016	151203	1.69%	0.309%
40	14.868	2170	2173	2178	rVB	297108	281253	3.14%	0.576%
41	15.051	2201	2204	2212	rVB	126686	242255	2.71%	0.496%
42	15.133	2214	2218	2221	rBV	138770	167912	1.88%	0.344%
43	15.415	2263	2266	2270	rVB	119868	135892	1.52%	0.278%
44	15.480	2272	2277	2281	rBV	1288541	1614424	18.03%	3.304%
45	15.515	2281	2283	2291	rVB2	148987	181074	2.02%	0.371%
46	15.951	2354	2357	2362	rVB	94777	122440	1.37%	0.251%

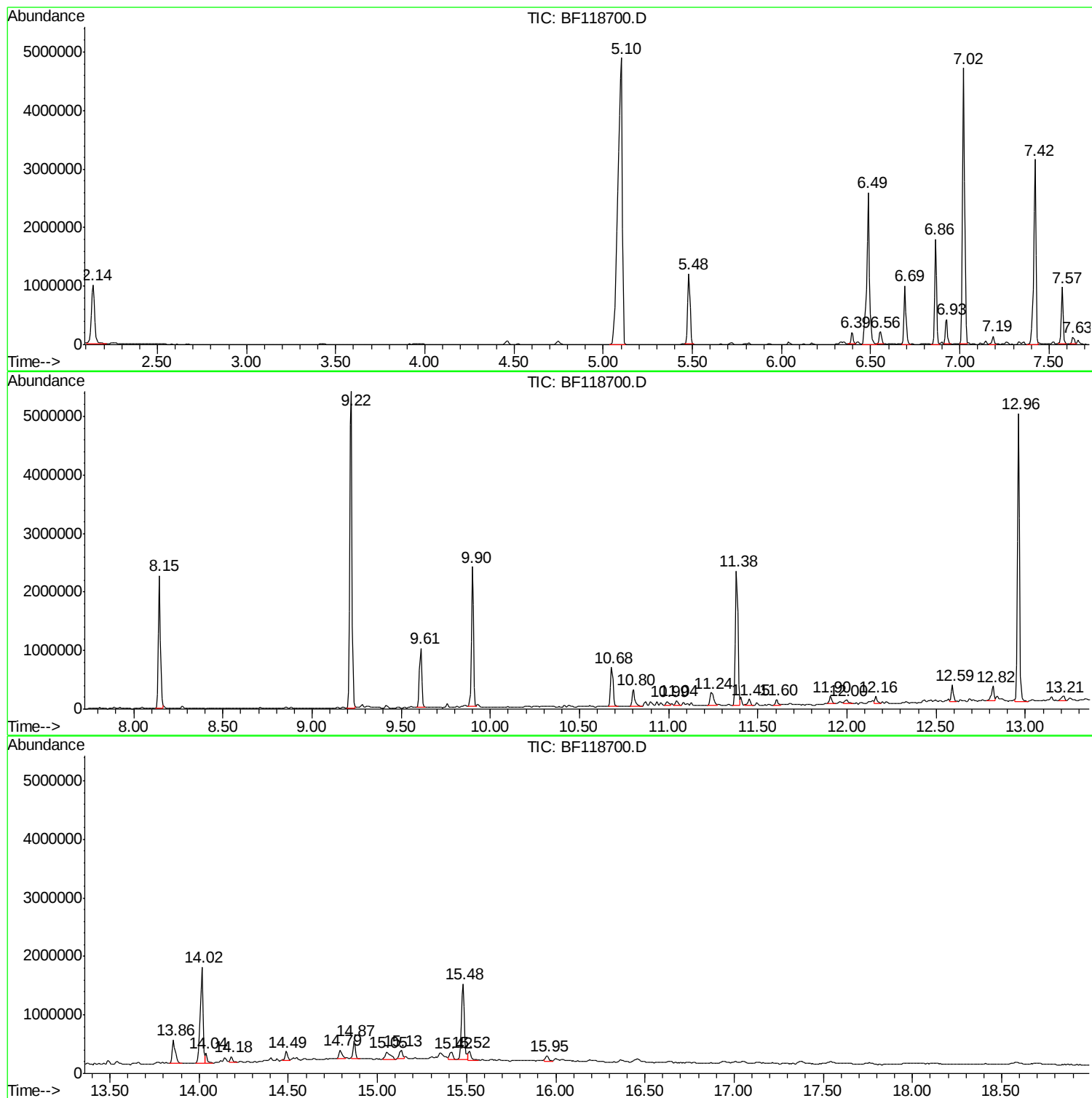
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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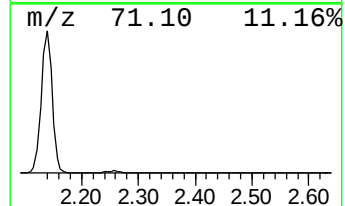
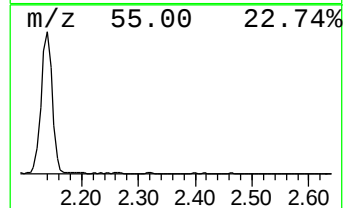
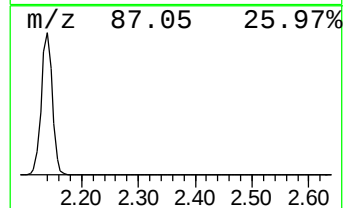
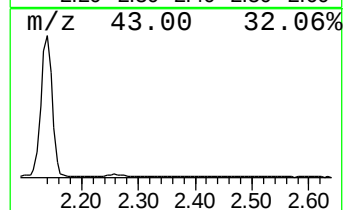
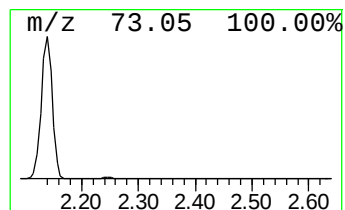
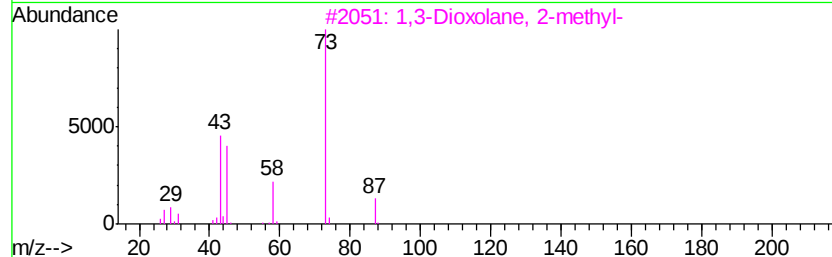
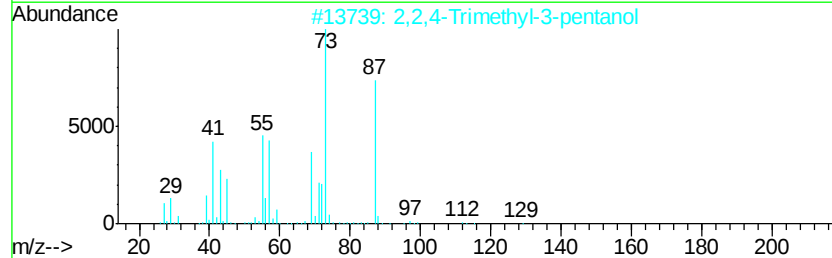
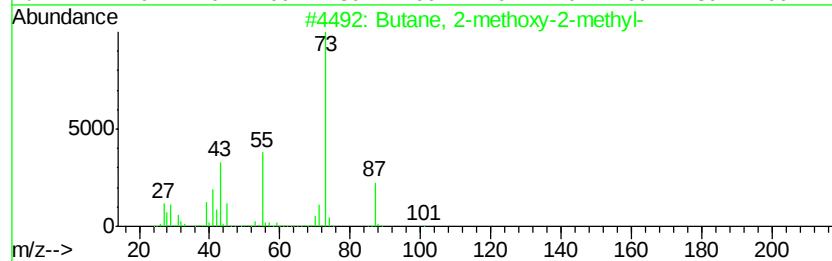
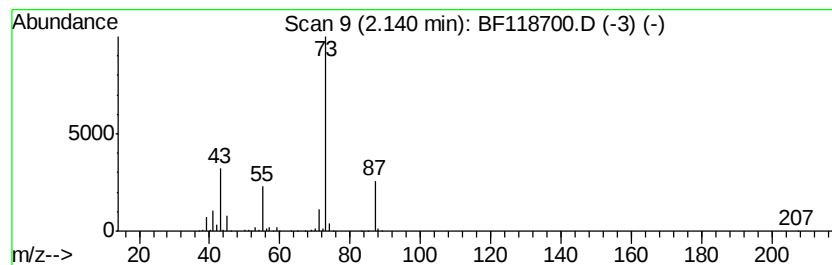
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	18.77 ng	1363520	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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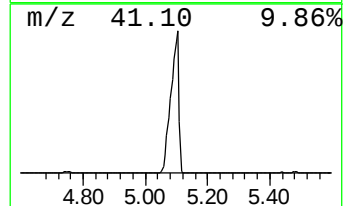
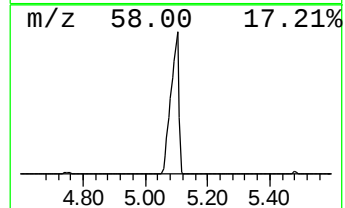
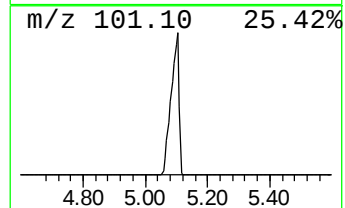
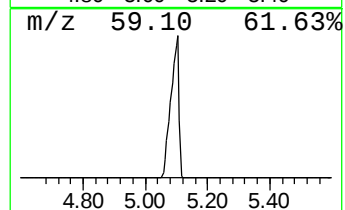
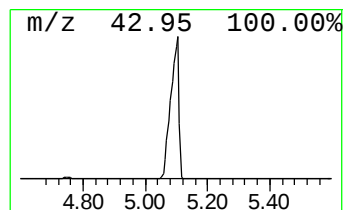
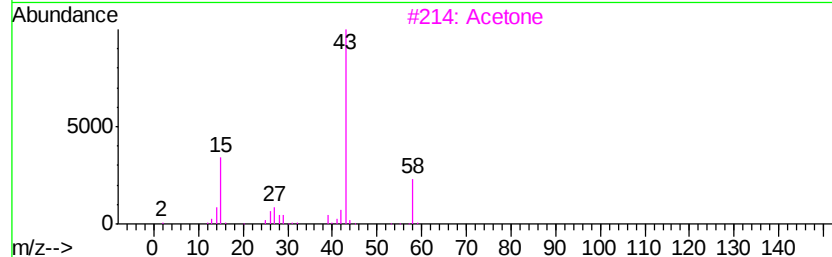
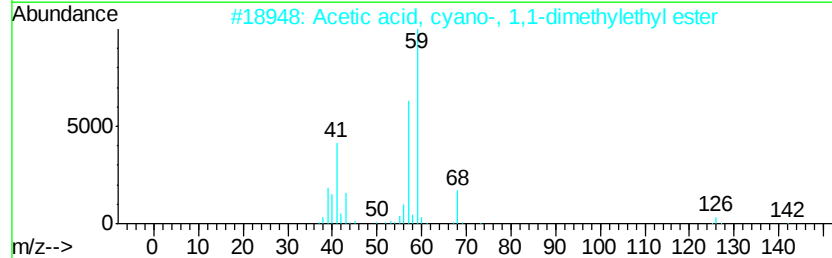
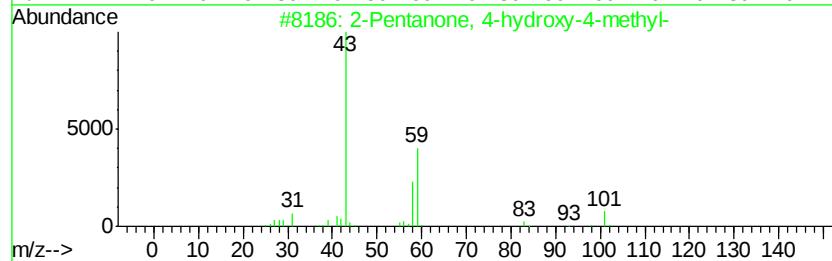
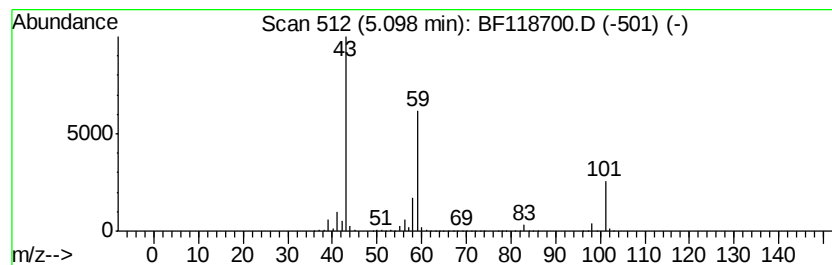
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	123.24 ng	8954040	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetone	58	C3H6O	000067-64-1	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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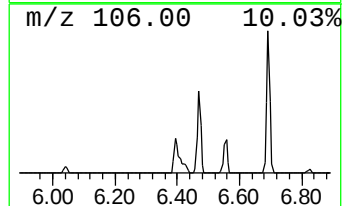
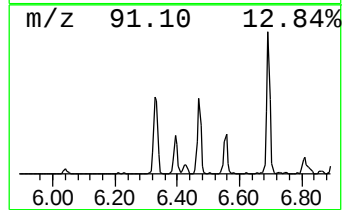
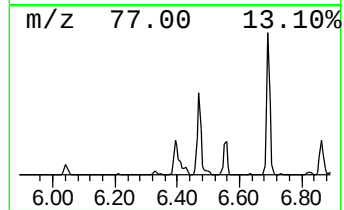
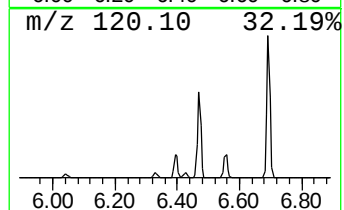
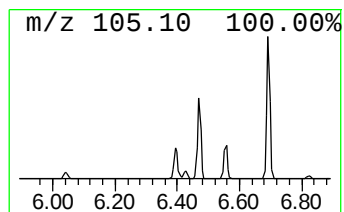
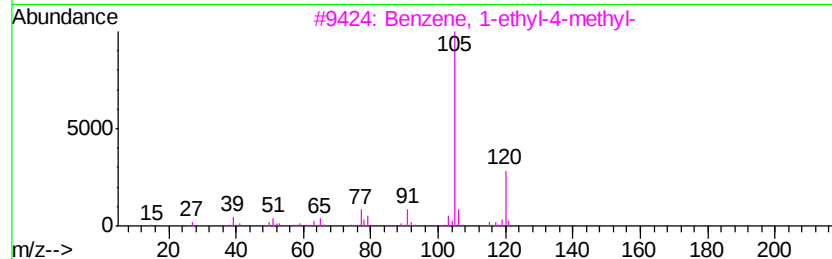
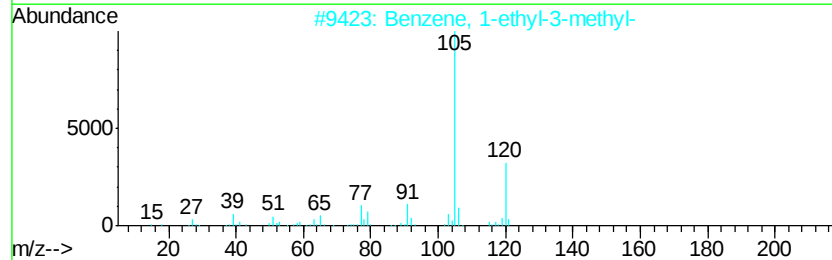
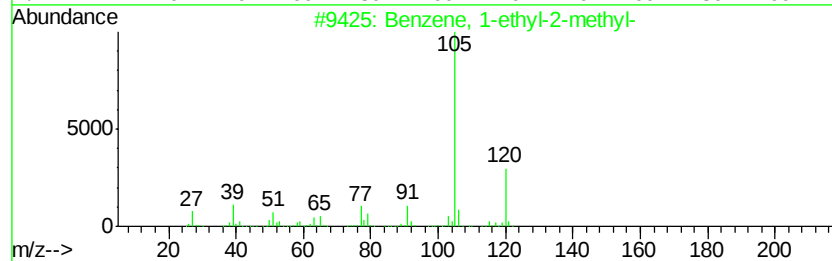
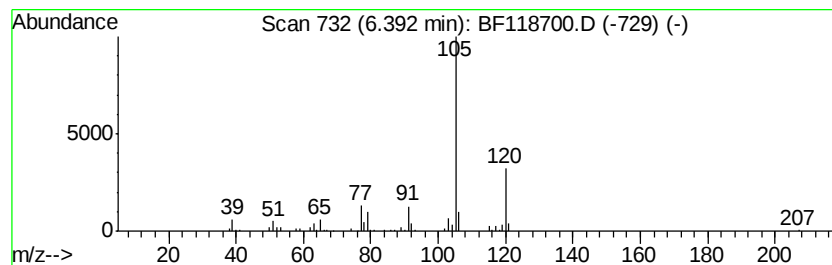
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	2.42 ng	175537	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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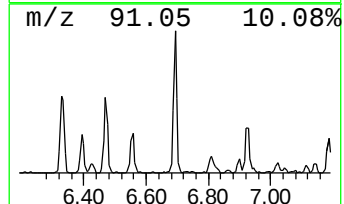
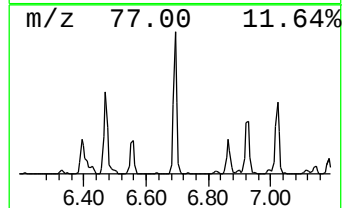
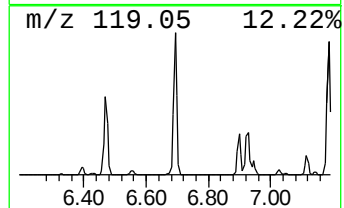
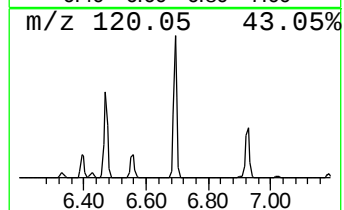
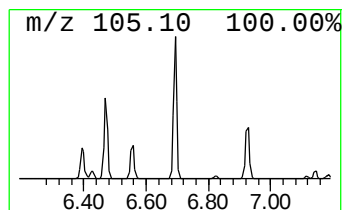
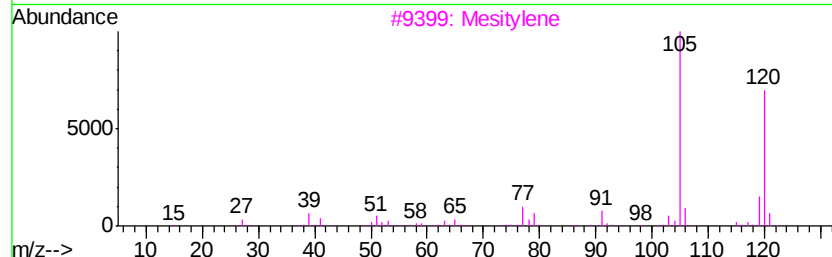
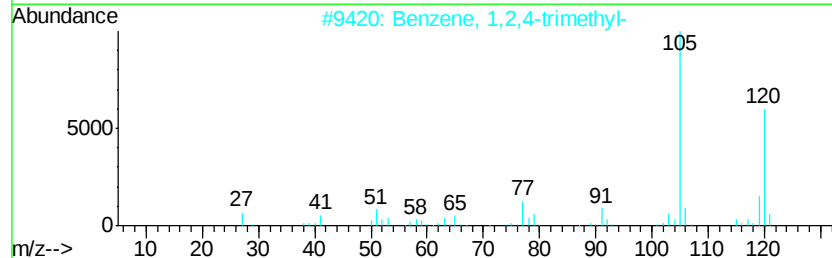
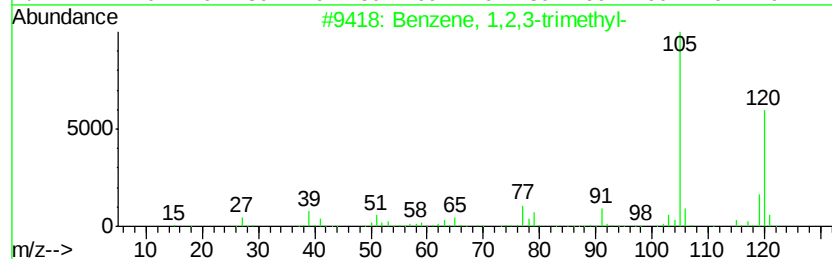
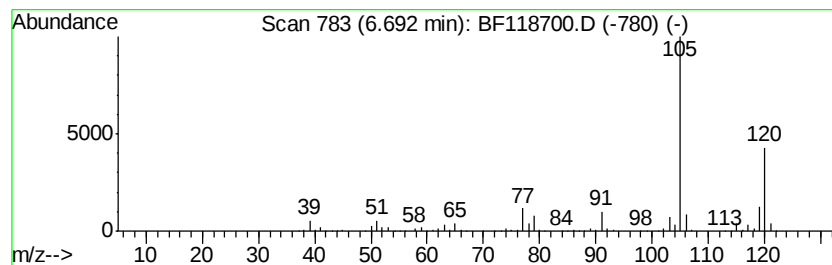
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	10.53 ng	765305	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3		Mesitylene	120	C9H12	000108-67-8	91
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



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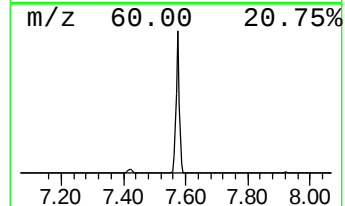
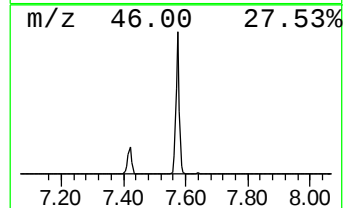
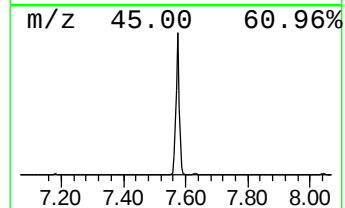
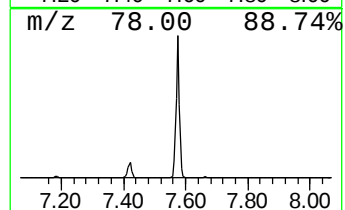
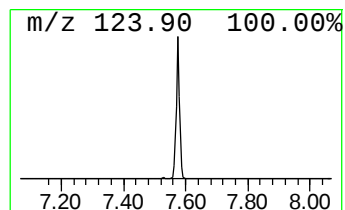
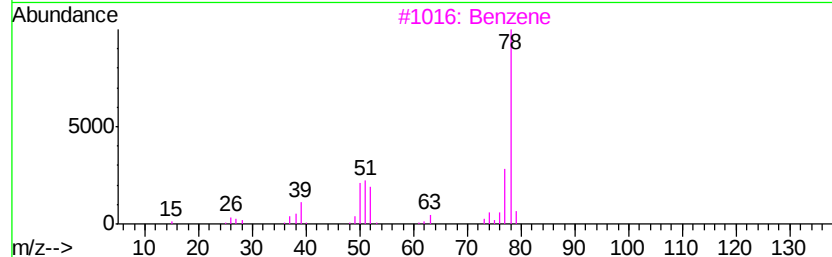
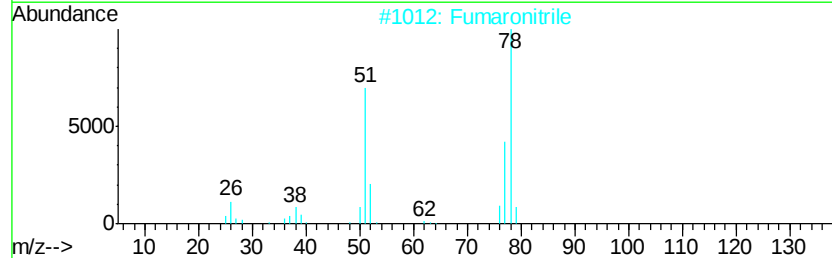
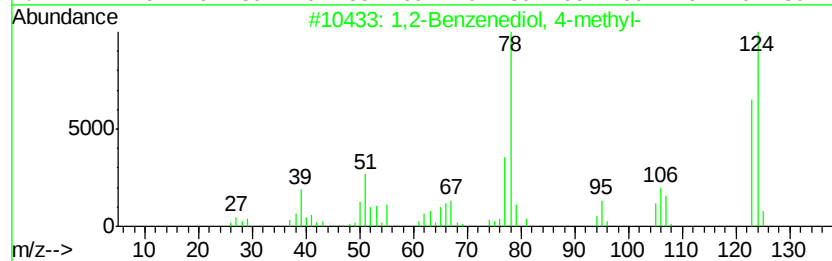
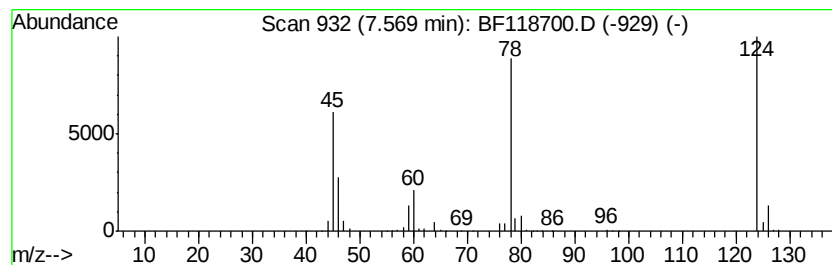
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,2-Benzenediol, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	8.40 ng	771671	Napthalene-d8	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	50
2		Fumaronitrile	78	C4H2N2	000764-42-1	9
3		Benzene	78	C6H6	000071-43-2	9
4		1,2,4-Trithiolane	124	C2H4S3	000289-16-7	9
5		Carbamothioic acid, O-butyl ester	133	C5H11NOS	000692-99-9	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
Data File : BF118700.D
Acq On : 24 Jan 2020 22:03
Operator : CG/JU
Sample : L1242-11
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
20200064-AMENDED-COMP-2

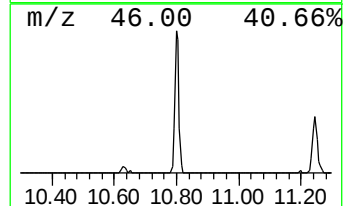
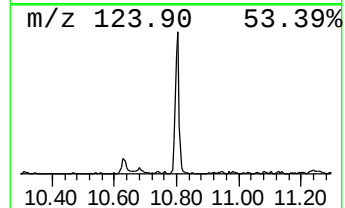
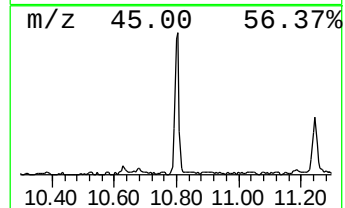
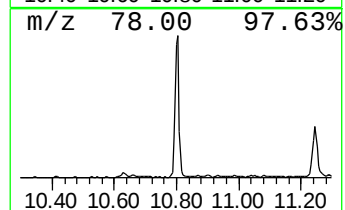
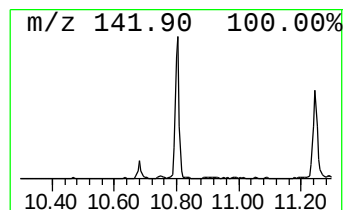
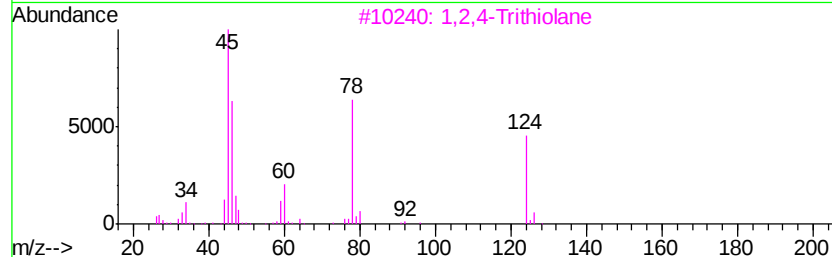
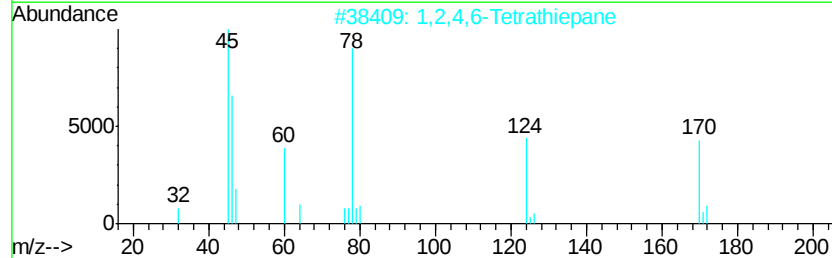
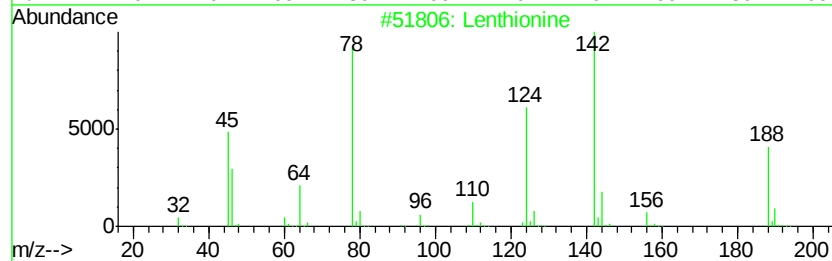
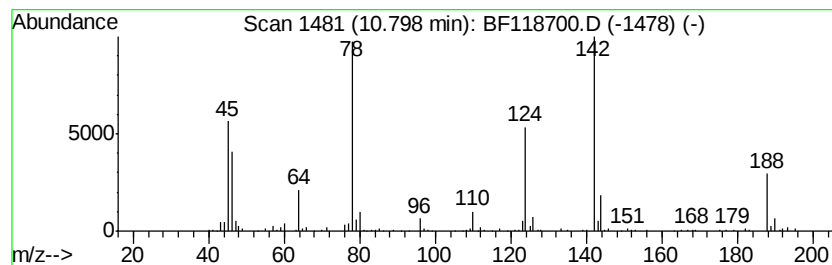
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Lenthionine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	3.34 ng	331206	Phenanthrene-d10	11.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Lenthionine	188	C2H4S5	000292-46-6	96
2		1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
3		1,2,4-Trithiolane	124	C2H4S3	000289-16-7	45
4		Ehylthiophosphonamide, o-methyl ...	139	C3H10NOPS	1000306-03-7	40
5		1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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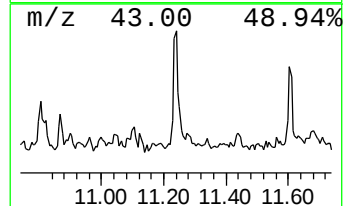
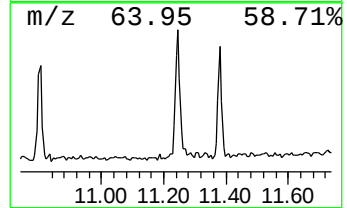
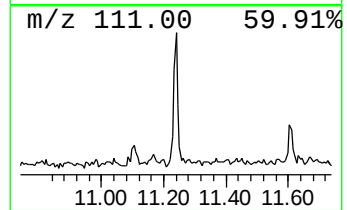
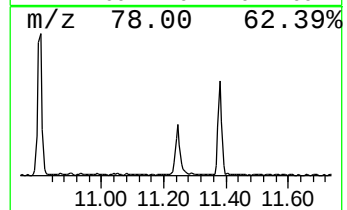
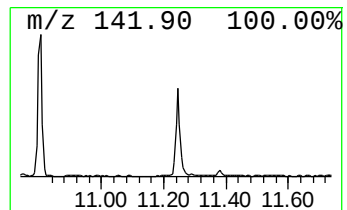
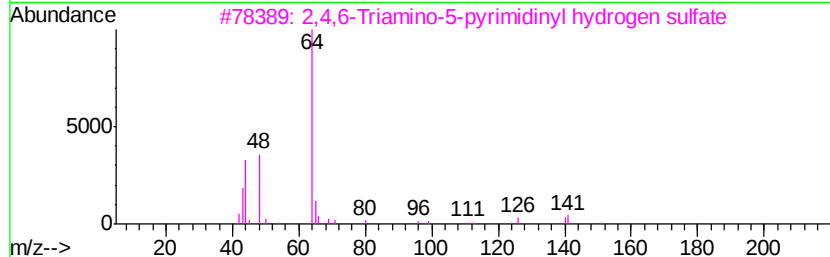
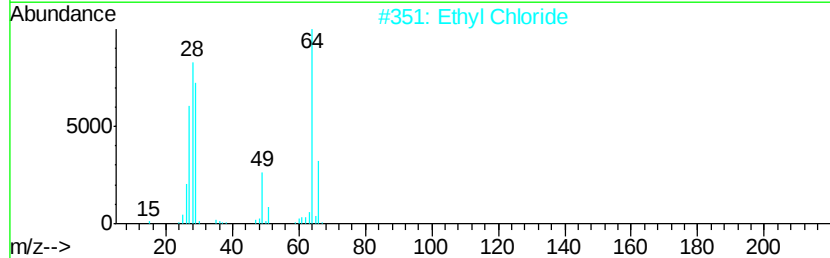
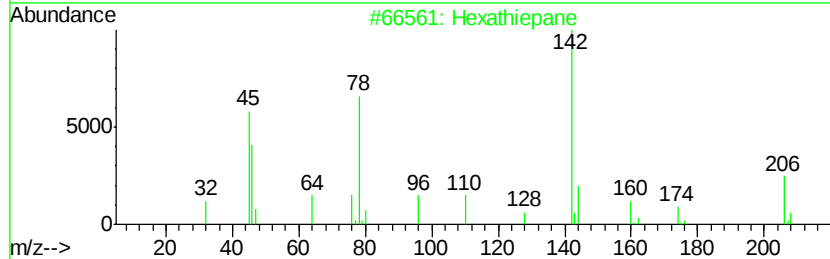
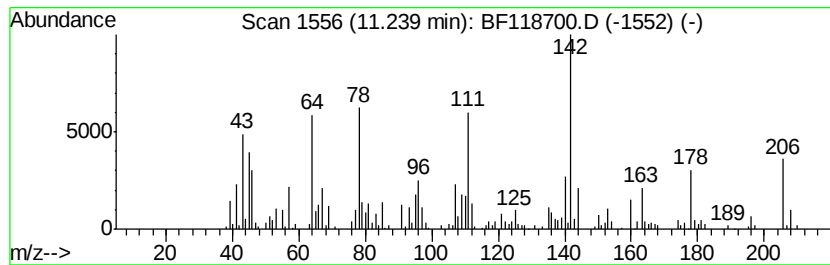
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexathiepane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	2.93 ng	290430	Phenanthrene-d10	11.38
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexathiepane	206	CH2S6	017233-71-5 59
2	Ethyl Chloride	64	C2H5Cl	000075-00-3 27
3	2,4,6-Triamino-5-pyrimidinyl hvd...	221	C4H7N5O4S	071552-23-3 16
4	1-[1-Bromo-2-(2,2,3,3-tetrafluor...	328	C12H10BrF5	1000223-18-3 16
5	6-Methoxyquinolinimide	178	C8H6N2O3	1000214-53-5 16



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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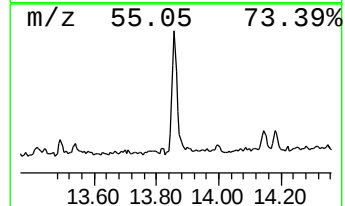
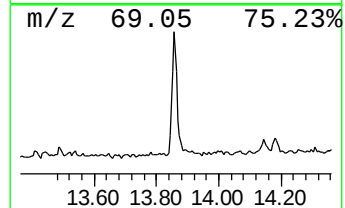
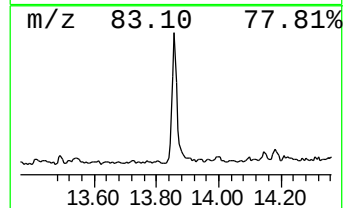
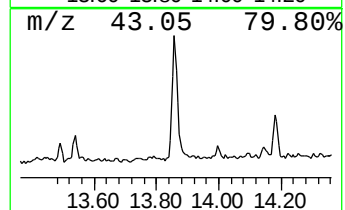
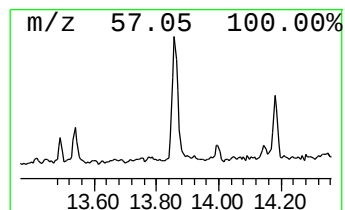
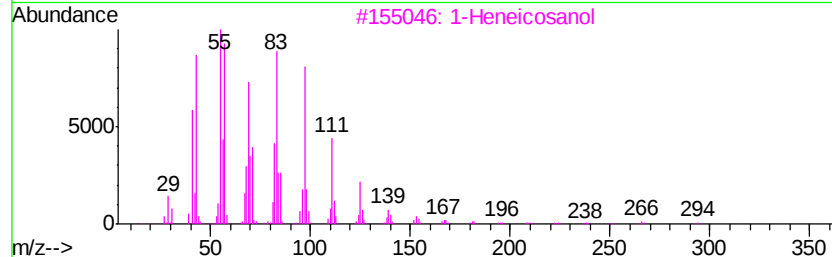
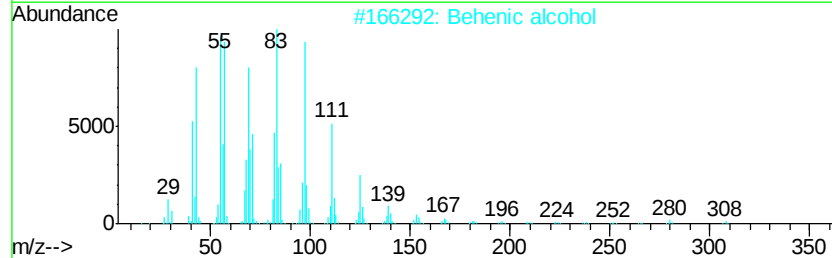
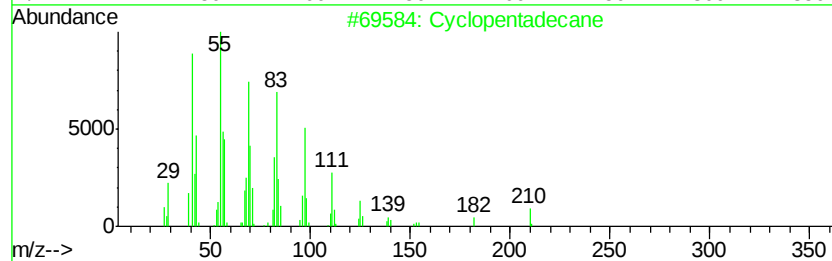
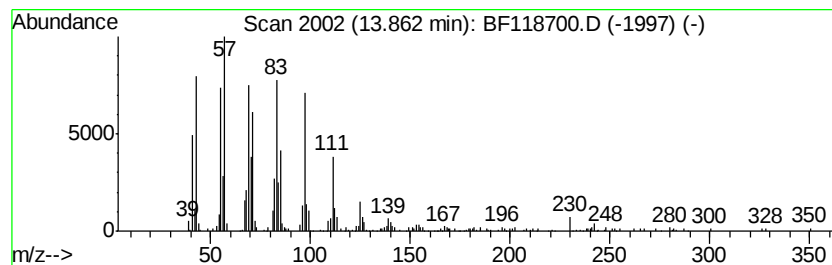
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	5.51 ng	472679	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentadecane	210	C15H30	000295-48-7	98
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		1-Heneicosanol	312	C21H44O	015594-90-8	94
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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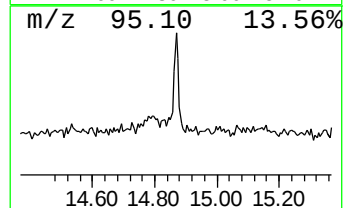
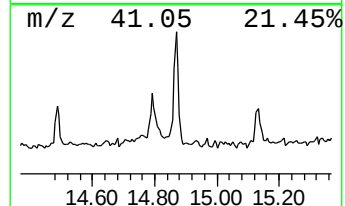
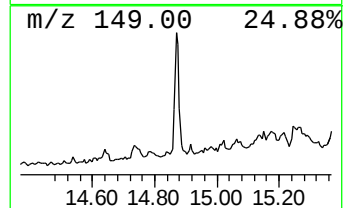
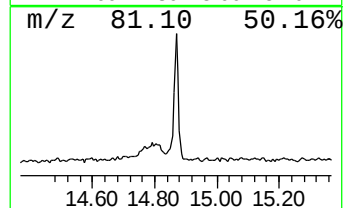
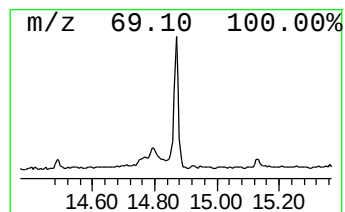
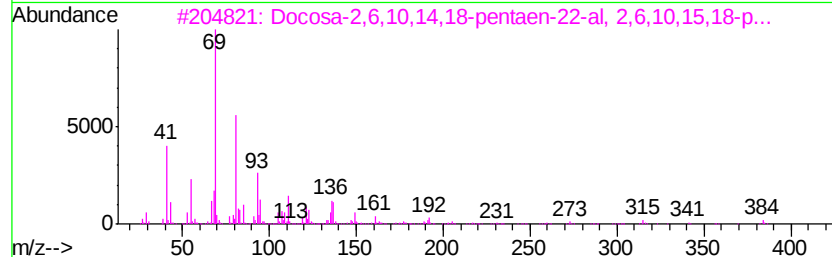
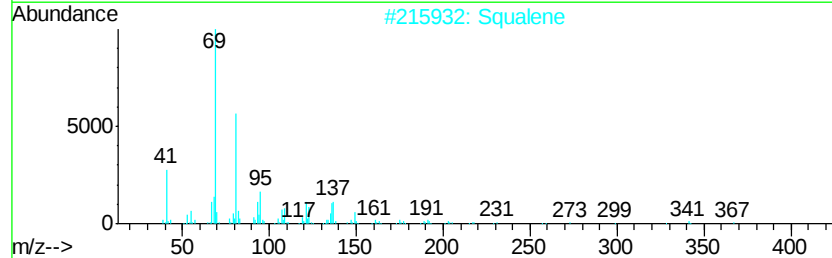
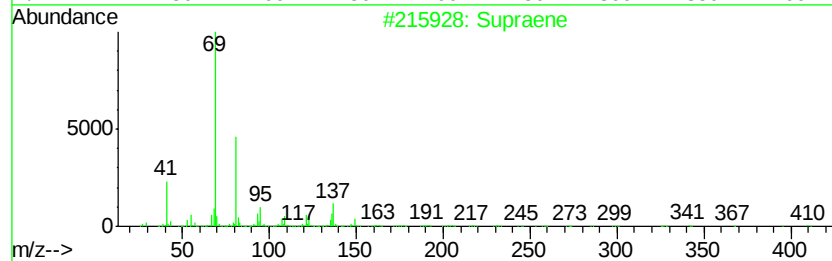
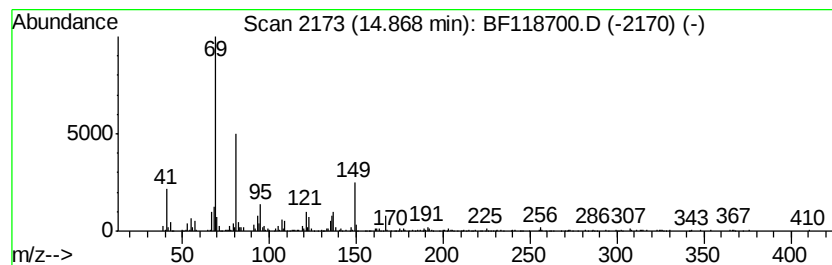
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.48 ng	281253	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	98
2		Squalene	410	C30H50	000111-02-4	81
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
4		2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	003675-00-1	53
5		2,6,10-Dodecatrienoic acid, 3,7,...	250	C16H26O2	004176-79-8	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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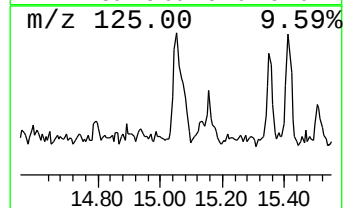
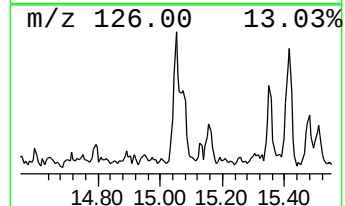
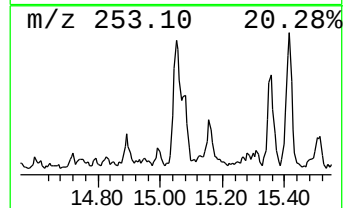
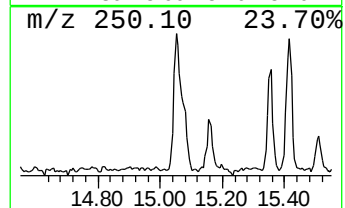
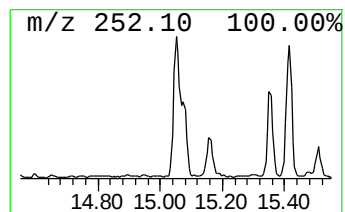
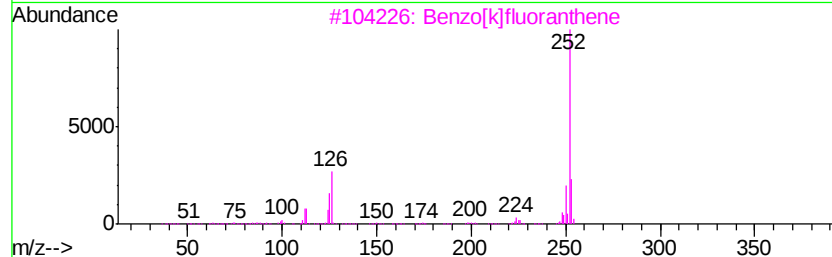
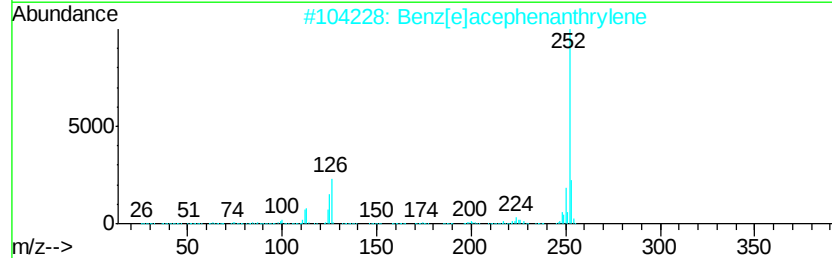
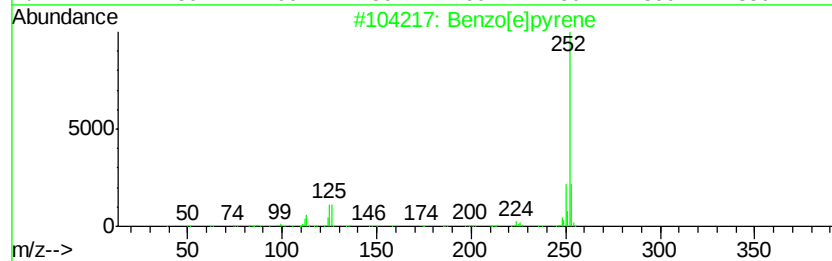
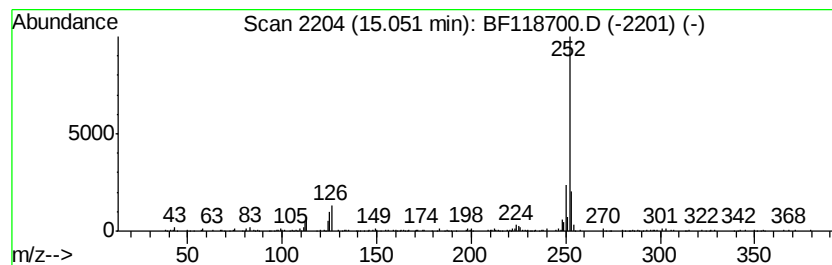
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.05	3.00 ng	242255	Perylene-d12	15.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzo[e]pyrene	252 C20H12	000192-97-2 98
2		Benzo[e]acephenanthrylene	252 C20H12	000205-99-2 95
3		Benzo[k]fluoranthene	252 C20H12	000207-08-9 93
4		Perylene	252 C20H12	000198-55-0 90
5		Benzo[a]pyrene	252 C20H12	000050-32-8 90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012420\
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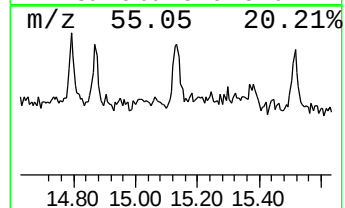
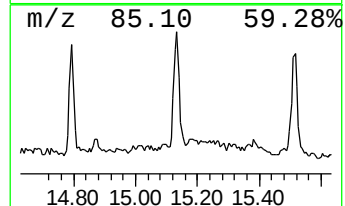
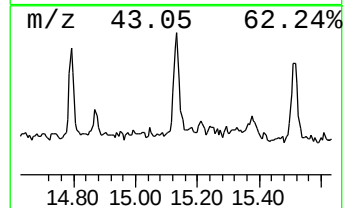
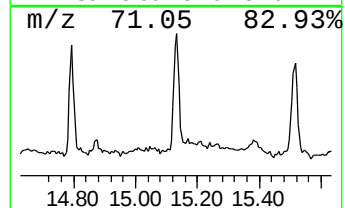
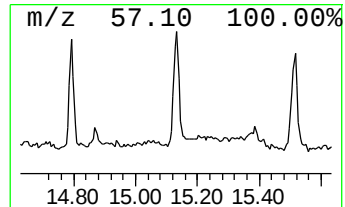
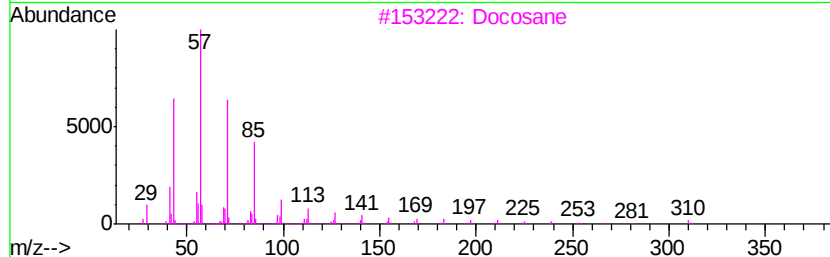
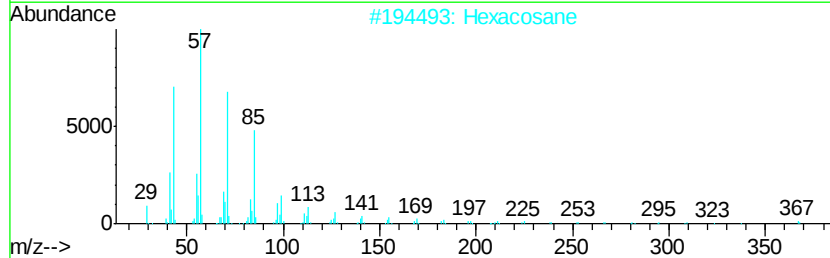
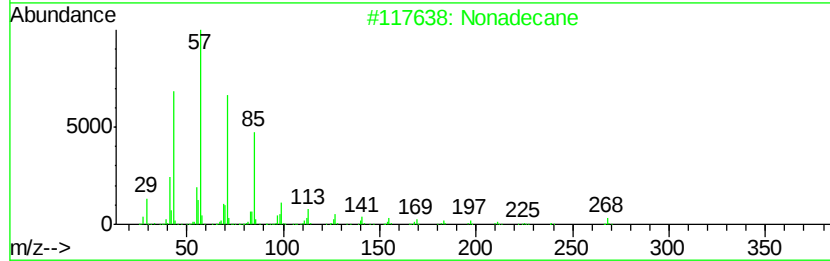
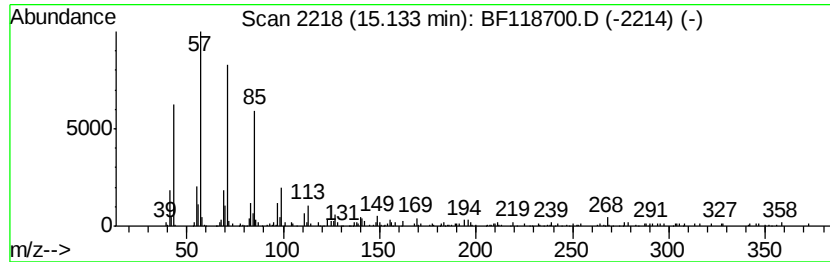
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Nonadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.13	2.08 ng	167912	Perylene-d12	15.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Hexacosane	366	C26H54	000630-01-3	87
3	Docosane	310	C22H46	000629-97-0	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012420\
 Data File : BF118700.D
 Acq On : 24 Jan 2020 22:03
 Operator : CG/JU
 Sample : L1242-11
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.14	18.8	ng	1363520	1	6.86	1453090	20.0
2-Pentanone, 4-hy...	5.10	123.2	ng	8954040	1	6.86	1453090	20.0
Benzene, 1-ethyl-...	6.39	2.4	ng	175537	1	6.86	1453090	20.0
Benzene, 1,2,3-tr...	6.69	10.5	ng	765305	1	6.86	1453090	20.0
1,2-Benzenediol, ...	7.57	8.4	ng	771671	2	8.15	1836600	20.0
Lenthionine	10.80	3.3	ng	331206	4	11.38	1980740	20.0
Hexathiepane	11.24	2.9	ng	290430	4	11.38	1980740	20.0
Cyclopentadecane	13.86	5.5	ng	472679	5	14.02	1716890	20.0
Supraene	14.87	3.5	ng	281253	6	15.48	1614420	20.0
Benzo[e]pyrene	15.05	3.0	ng	242255	6	15.48	1614420	20.0
Nonadecane	15.13	2.1	ng	167912	6	15.48	1614420	20.0