

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062921\
 Data File : BP006102.D
 Acq On : 29 Jun 2021 21:27
 Operator : CG/JU
 Sample : M2885-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 41547

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_P\Methods\8270E-BP060821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006102.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.011	323	327	337	rBV	24469	38553	1.17%	0.133%
2	5.475	400	406	424	rBV	1281336	1985724	60.27%	6.826%
3	7.081	672	679	696	rBV	1083417	1858898	56.42%	6.390%
4	7.899	807	818	827	rBV	362447	591188	17.94%	2.032%
5	9.069	1009	1017	1032	rBV	692006	1192817	36.20%	4.101%
6	10.499	1253	1260	1272	rBV	48443	110933	3.37%	0.381%
7	10.705	1286	1295	1300	rBV	397095	690066	20.94%	2.372%
8	10.752	1300	1303	1310	rVB	100697	165103	5.01%	0.568%
9	11.563	1431	1441	1448	rBV2	16250	43577	1.32%	0.150%
10	12.363	1571	1577	1588	rBV	92459	152938	4.64%	0.526%
11	12.581	1609	1614	1619	rVB	46631	70765	2.15%	0.243%
12	13.157	1705	1712	1724	rBV	1674925	2404090	72.96%	8.265%
13	13.369	1743	1748	1753	rBV	39061	65384	1.98%	0.225%
14	13.716	1798	1807	1813	rBV2	38580	108086	3.28%	0.372%
15	13.857	1825	1831	1835	rBV	58564	112108	3.40%	0.385%
16	13.910	1836	1840	1844	rVB2	28830	43154	1.31%	0.148%
17	14.257	1895	1899	1905	rBV2	35677	61303	1.86%	0.211%
18	14.357	1912	1916	1921	rVB4	27057	41981	1.27%	0.144%
19	14.534	1935	1946	1951	rBV	536834	915730	27.79%	3.148%
20	14.593	1951	1956	1965	rVB	304947	484687	14.71%	1.666%
21	14.845	1995	1999	2004	rBV2	26172	44658	1.36%	0.154%
22	14.928	2008	2013	2023	rVB	222183	351217	10.66%	1.207%
23	15.310	2074	2078	2083	rBV4	73135	129623	3.93%	0.446%
24	15.575	2118	2123	2129	rBV	433702	695222	21.10%	2.390%
25	15.740	2148	2151	2156	rVB2	52509	71941	2.18%	0.247%
26	15.869	2170	2173	2180	rVB	75709	110282	3.35%	0.379%
27	16.022	2194	2199	2206	rBV	1472067	2161714	65.61%	7.431%
28	17.281	2408	2413	2416	rBV	662085	947218	28.75%	3.256%
29	17.322	2416	2420	2427	rVB	1518201	2109768	64.03%	7.253%
30	17.416	2432	2436	2441	rVB	363017	507153	15.39%	1.743%
31	19.286	2749	2754	2759	rBV	1164126	1526059	46.32%	5.246%
32	19.604	2805	2808	2810	rBV2	196293	260738	7.91%	0.896%
33	19.633	2810	2813	2821	rVB	831135	1225683	37.20%	4.214%
34	19.828	2841	2846	2850	rVB	2850699	3294934	100.00%	11.327%
35	20.210	2909	2911	2915	rVB	130457	145557	4.42%	0.500%
36	20.980	3039	3042	3044	rBV2	136563	166161	5.04%	0.571%

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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_P\Methods\8270E-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.010	3044	3047	3050	rVV2	201101	268127	8.14%	0.922%
38	21.051	3050	3054	3057	rVB2	255781	337559	10.24%	1.160%
39	21.351	3099	3105	3109	rBV2	1072230	1836075	55.72%	6.312%
40	21.386	3109	3111	3118	rVB	359793	475617	14.43%	1.635%
41	23.757	3508	3514	3520	rBV2	669956	1286229	39.04%	4.422%

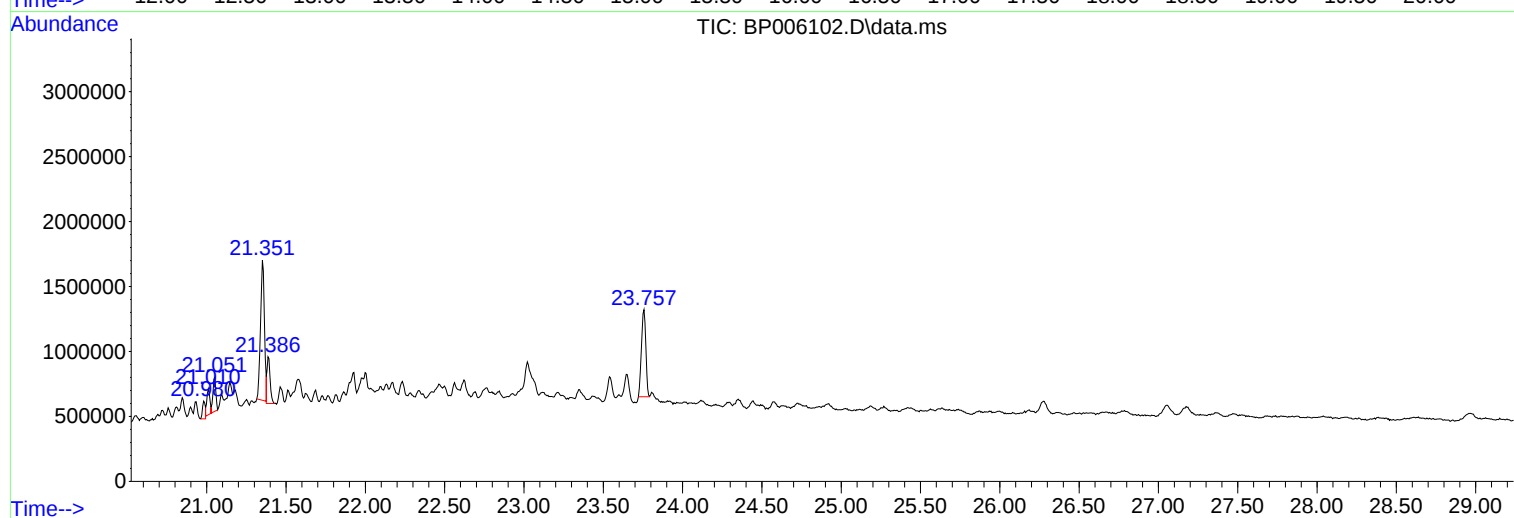
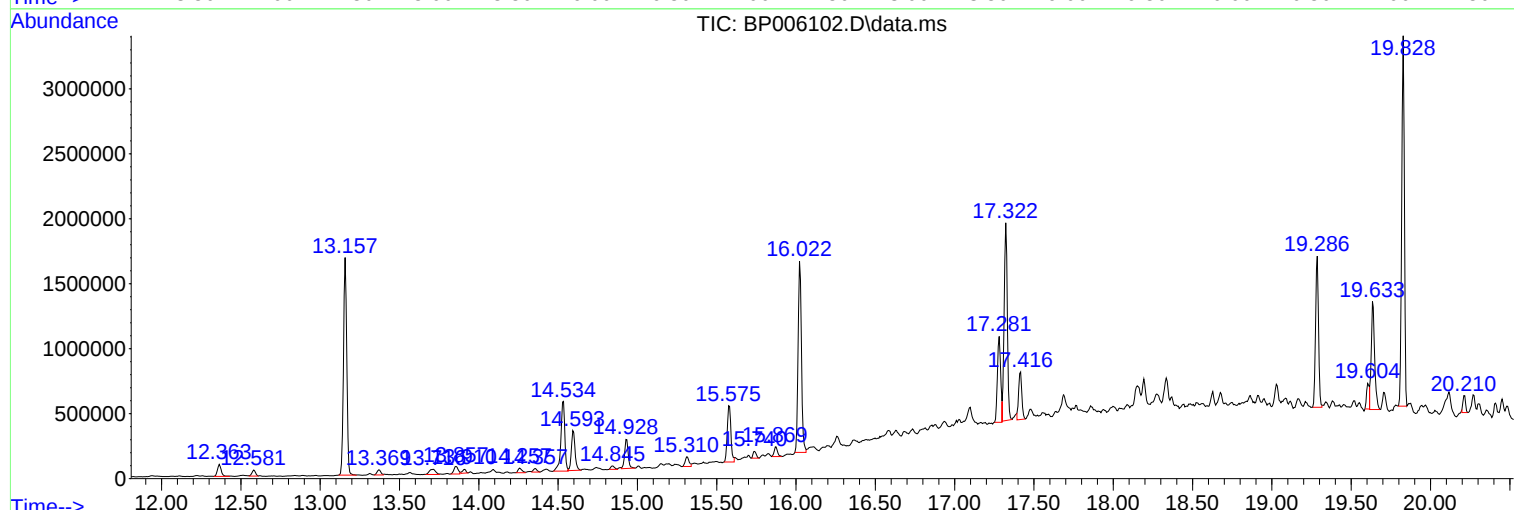
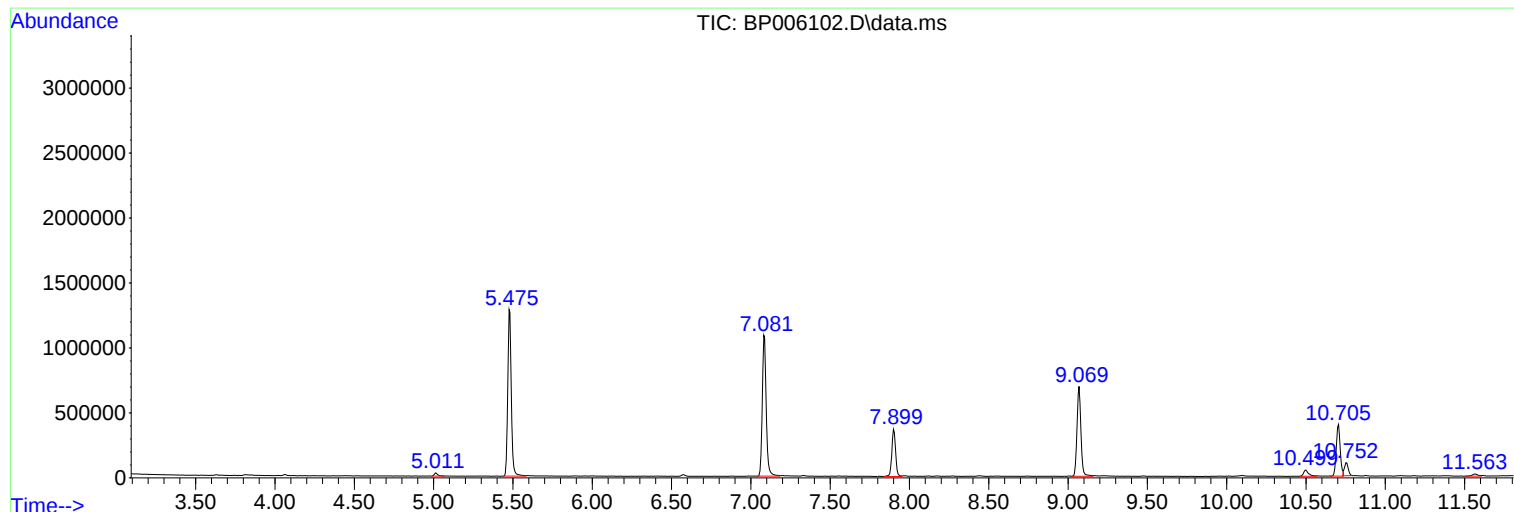
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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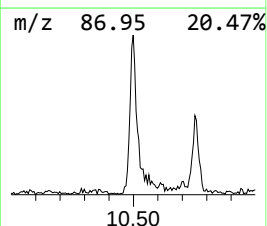
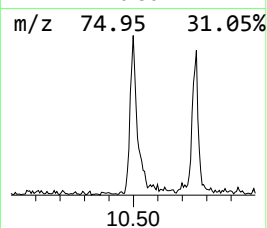
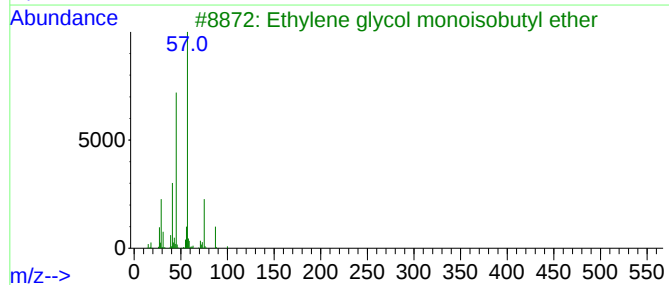
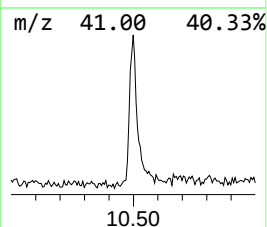
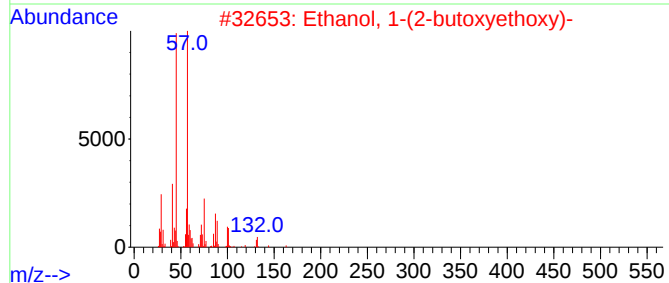
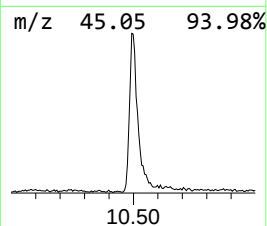
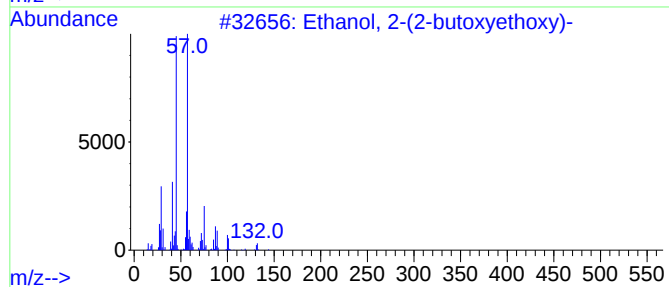
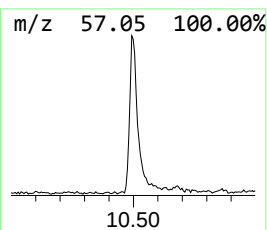
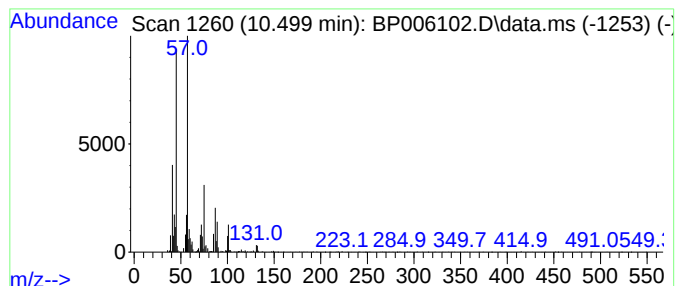
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.499	3.22 ng	110933	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	53
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53



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ALS Vial : 14 Sample Multiplier: 1

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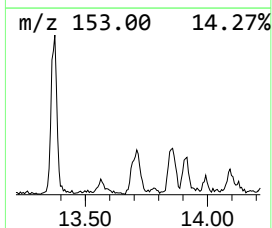
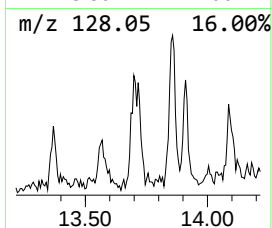
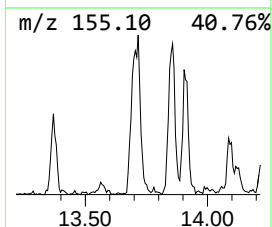
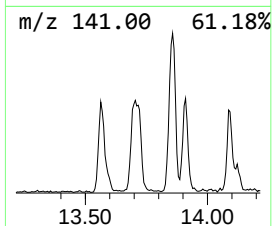
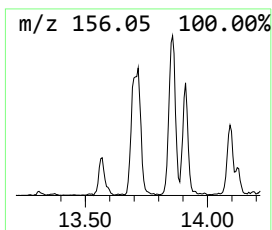
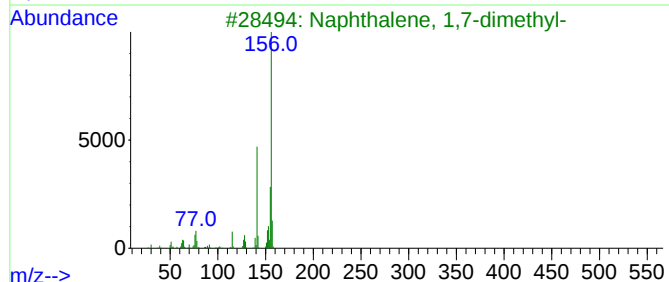
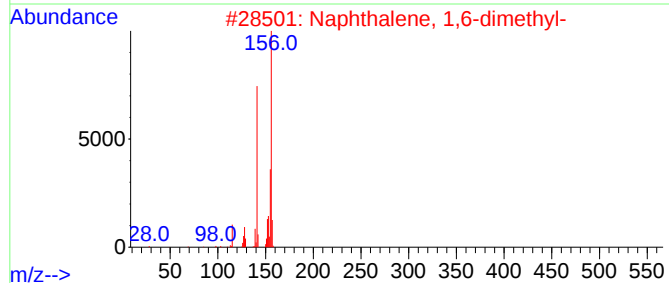
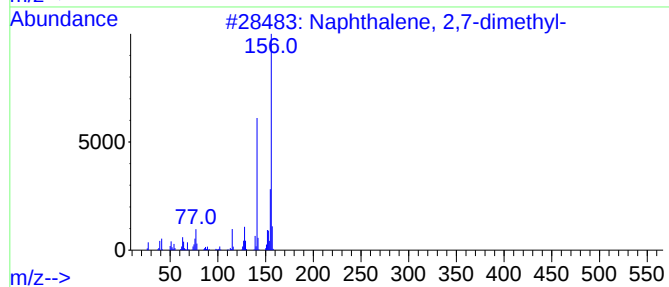
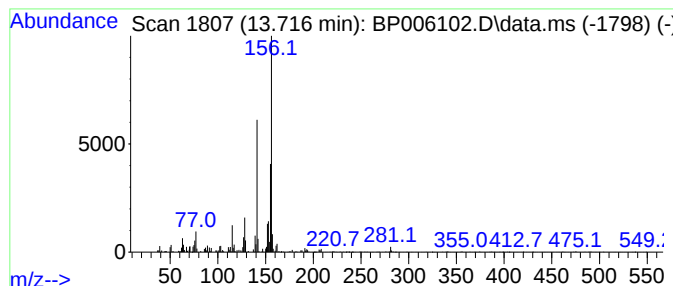
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Naphthalene, 2,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.716	2.36 ng	108086	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	91
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	90
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	90
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	86



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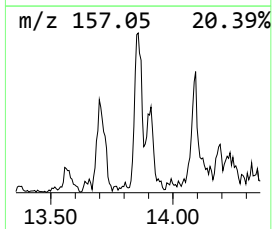
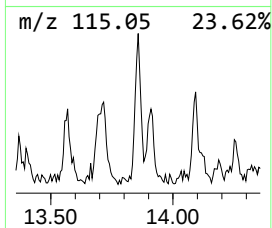
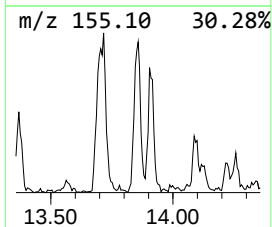
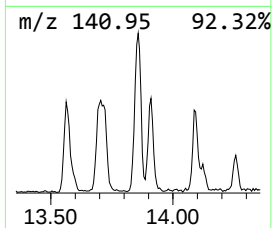
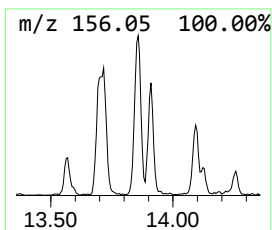
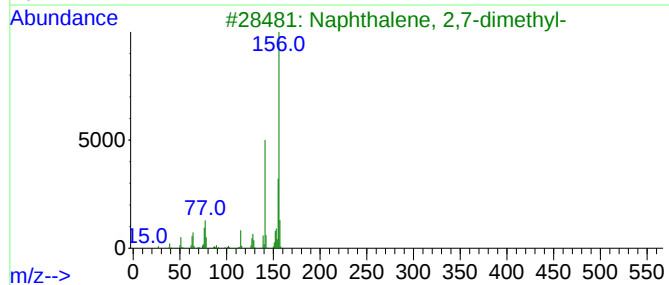
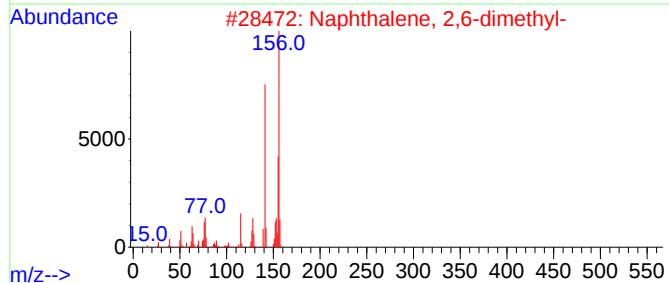
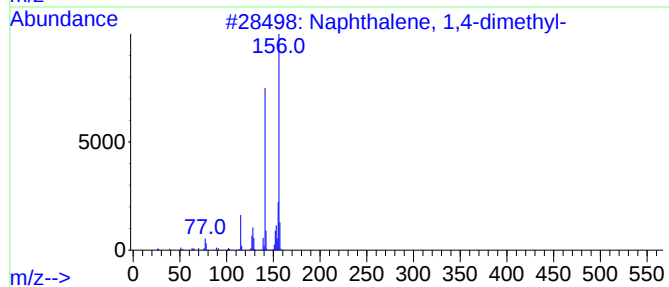
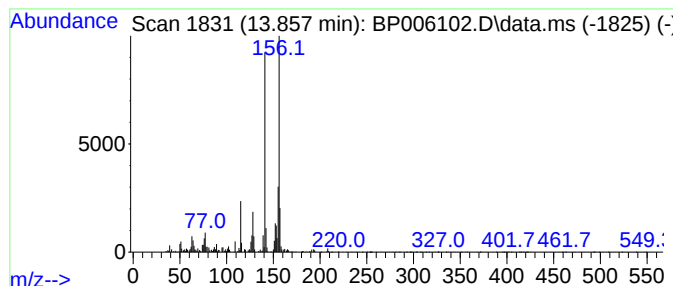
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 1,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	2.45 ng	112108	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	95
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	94
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	93
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	93



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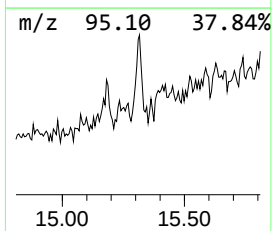
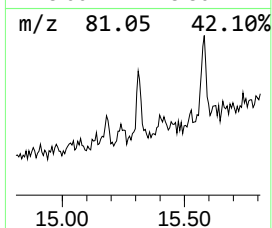
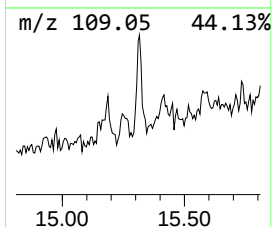
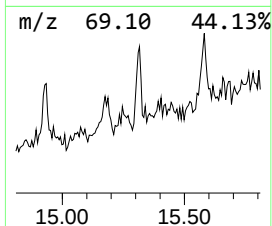
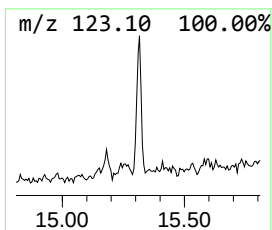
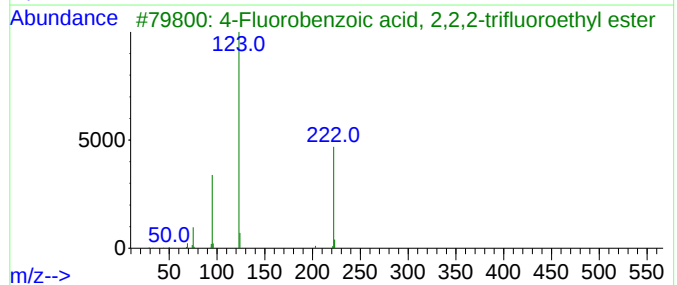
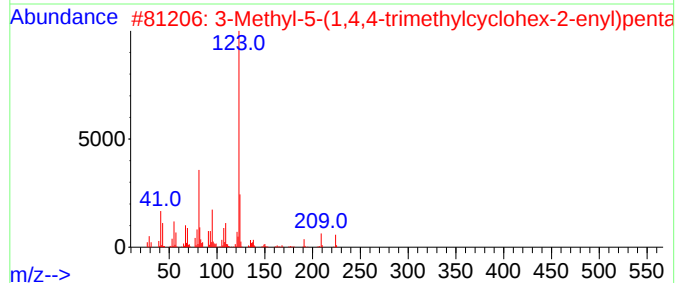
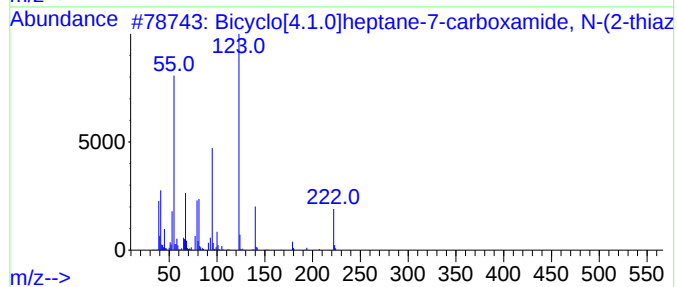
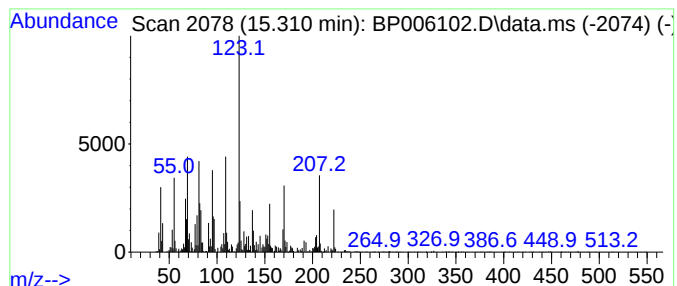
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown15.310 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.310	2.83 ng	129623	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2O5	329912-72-3	41
2			3-Methyl-5-(1,4,4-trimethylcyclo...	224	C15H28O	1000187-09-1	38
3			4-Fluorobenzoic acid, 2,2,2-trif...	222	C9H6F4O2	1000325-53-2	38
4			2-Fluoro-N-(4-methyl-thiazol-2-y...	236	C11H9FN2O5	325778-72-1	30
5			3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	30



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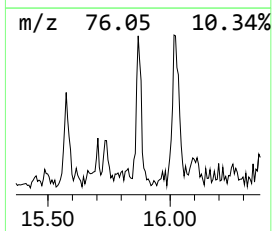
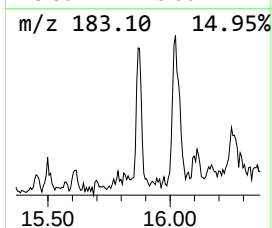
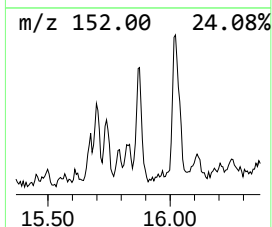
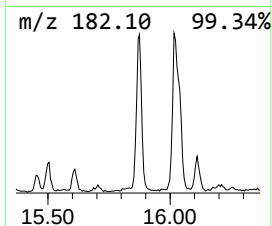
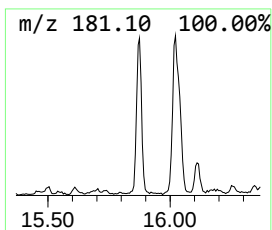
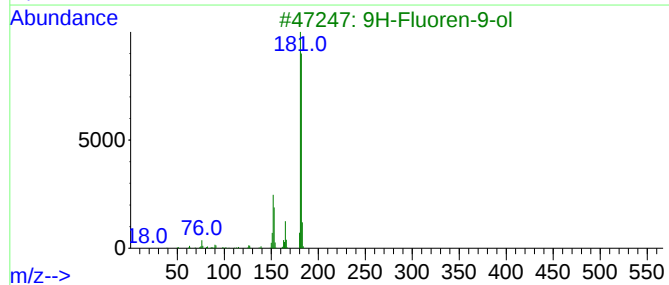
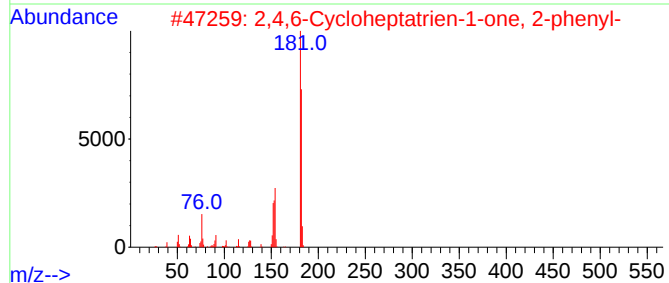
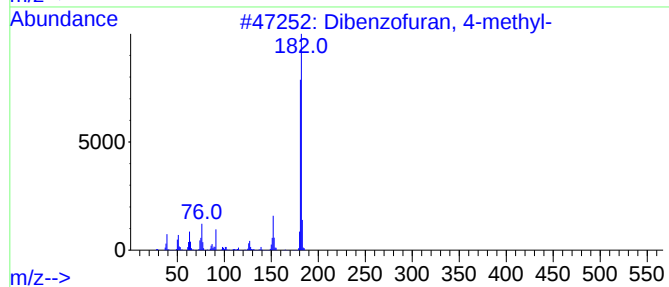
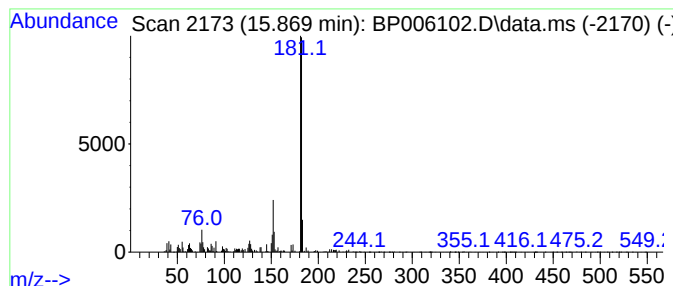
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dibenzofuran, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.869	2.41 ng	110282	Acenaphthene-d10	14.534

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzofuran, 4-methyl-	182	C13H10O	007320-53-8	90
2			2,4,6-Cycloheptatrien-1-one, 2-p...	182	C13H10O	014562-09-5	80
3			9H-Fluoren-9-ol	182	C13H10O	001689-64-1	78
4			[1,1'-Biphenyl]-4-carboxaldehyde	182	C13H10O	003218-36-8	78
5			2-Hydroxyfluorene	182	C13H10O	002443-58-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062921\
Data File : BP006102.D
Acq On : 29 Jun 2021 21:27
Operator : CG/JU
Sample : M2885-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
41547

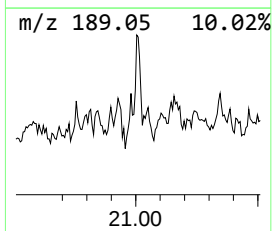
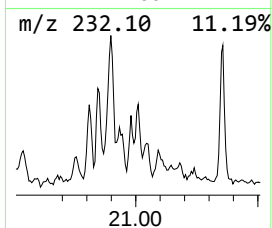
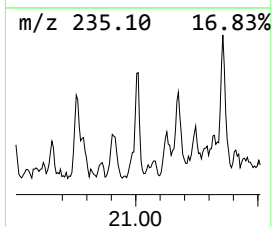
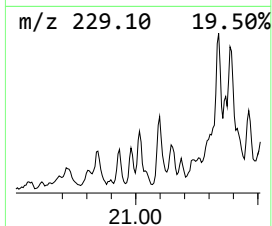
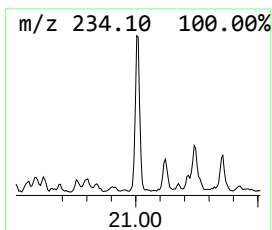
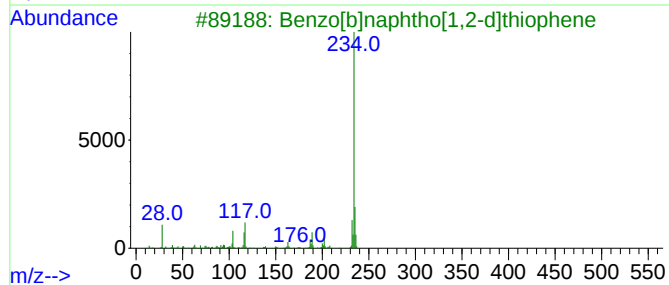
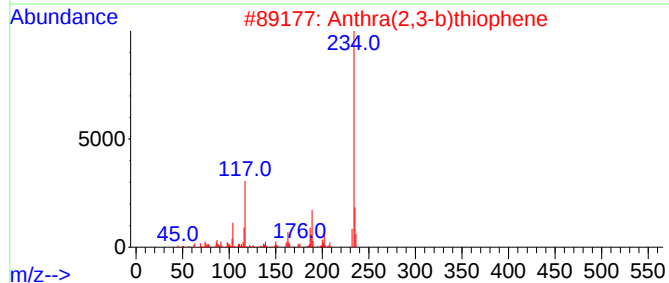
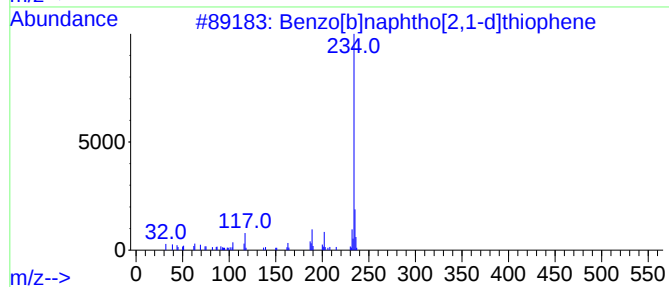
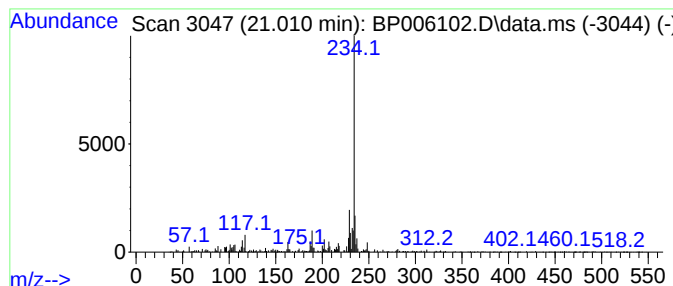
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[b]naphtho[2,1-d]thiop... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	2.92 ng	268127	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	89
2			Anthra(2,3-b)thiophene	234	C16H10S	022108-55-0	83
3			Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	83
4			Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	58
5			2,4-Diamino-5,6,7,8-tetrahydro-9...	234	C11H14N4S	042159-81-9	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062921\
Data File : BP006102.D
Acq On : 29 Jun 2021 21:27
Operator : CG/JU
Sample : M2885-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
41547

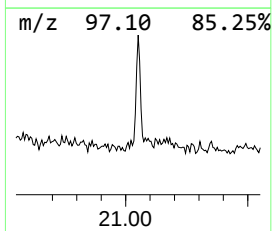
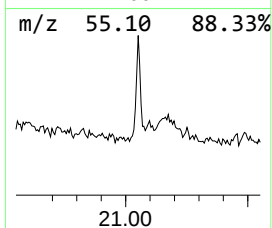
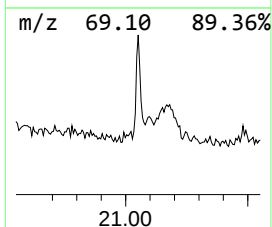
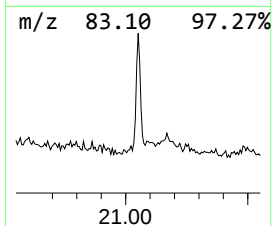
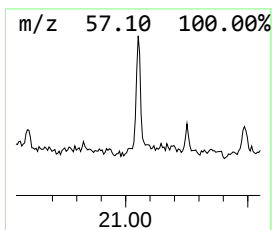
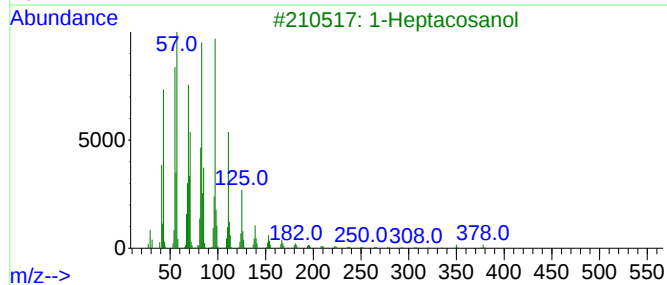
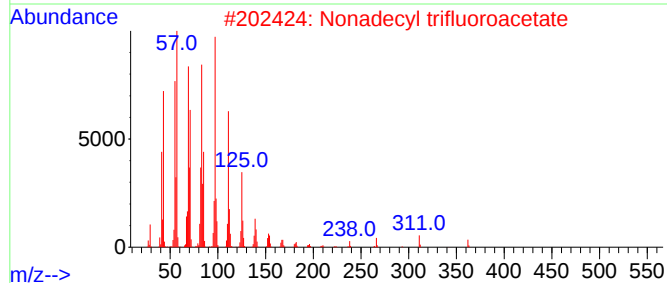
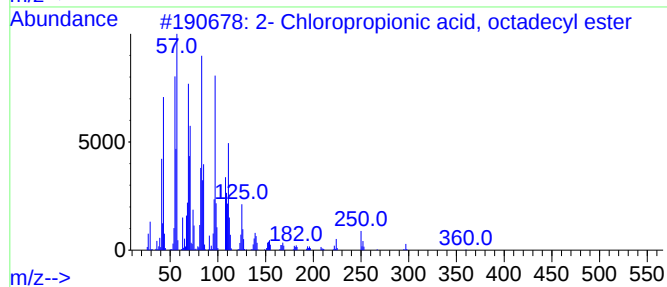
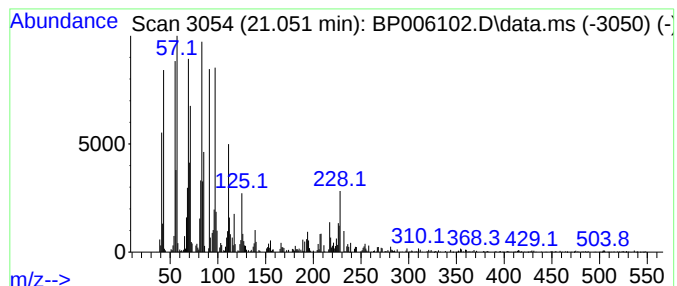
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2- Chloropropionic acid, oc... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	3.68 ng	337559	Chrysene-d12	21.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91	
2	Nonadecyl	trifluoroacetate	380	C21H39F3O2	1000351-76-3	91	
3	1-Heptacosanol		396	C27H56O	002004-39-9	91	
4	Heptafluorobutyric acid, pentade...		424	C19H31F7O2	959261-23-5	90	
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	90	



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062921\
Data File : BP006102.D
Acq On : 29 Jun 2021 21:27
Operator : CG/JU
Sample : M2885-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
41547

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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
Ethanol, 2-(2-b...	10.499	3.2	ng	110933	2	10.704	690066	20.0
Naphthalene, 2,...	13.716	2.4	ng	108086	3	14.534	915730	20.0
Naphthalene, 1,...	13.857	2.5	ng	112108	3	14.534	915730	20.0
unknown15.310	15.310	2.8	ng	129623	3	14.534	915730	20.0
Dibenzofuran, 4...	15.869	2.4	ng	110282	3	14.534	915730	20.0
Benzo[b]naphtho...	21.010	2.9	ng	268127	5	21.351	1836080	20.0
2- Chloropropio...	21.051	3.7	ng	337559	5	21.351	1836080	20.0