

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
 Data File : BF132271.D
 Acq On : 01 Feb 2023 21:07
 Operator : CG\JU
 Sample : 01357-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-205

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-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132271.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.307	415	420	431	rVB	1065981	1309322	35.05%	4.277%
2	5.690	480	485	488	rBV	3128492	3136151	83.95%	10.245%
3	6.678	648	653	656	rVB	2899325	3096218	82.88%	10.115%
4	6.731	659	662	674	rVB	30505	53072	1.42%	0.173%
5	7.066	716	719	723	rBV	1180156	953252	25.52%	3.114%
6	7.631	810	815	818	rBV	2460766	2084768	55.81%	6.811%
7	8.354	934	938	941	rBV	1689180	1278052	34.21%	4.175%
8	9.366	1103	1110	1112	rBV2	51461	63177	1.69%	0.206%
9	9.431	1117	1121	1124	rBV	4555987	3735686	100.00%	12.204%
10	9.513	1124	1135	1137	rVV2	37094	46898	1.26%	0.153%
11	9.825	1185	1188	1191	rBV	172235	155667	4.17%	0.509%
12	9.984	1211	1215	1217	rBV	98535	96923	2.59%	0.317%
13	10.031	1220	1223	1225	rVB	72350	65013	1.74%	0.212%
14	10.119	1234	1238	1241	rVB	1749314	1357780	36.35%	4.436%
15	10.148	1241	1243	1247	rBV5	39374	53411	1.43%	0.174%
16	10.295	1266	1268	1270	rBV	81723	61806	1.65%	0.202%
17	10.360	1276	1279	1288	rVB3	71675	99974	2.68%	0.327%
18	10.531	1305	1308	1311	rVB2	97045	91382	2.45%	0.299%
19	10.566	1312	1314	1317	rBV2	57938	64723	1.73%	0.211%
20	10.754	1343	1346	1350	rBV	442733	454773	12.17%	1.486%
21	10.831	1357	1359	1362	rVB	203356	151335	4.05%	0.494%
22	10.913	1369	1373	1376	rBV	2451337	2143148	57.37%	7.001%
23	10.954	1378	1380	1382	rVB	92617	74429	1.99%	0.243%
24	11.025	1389	1392	1395	rBV	899829	776826	20.79%	2.538%
25	11.236	1425	1428	1431	rBV2	206598	240128	6.43%	0.784%
26	11.495	1468	1472	1475	rBV	793186	744343	19.93%	2.432%
27	11.619	1489	1493	1496	rBV	1478715	1298542	34.76%	4.242%
28	11.642	1496	1497	1500	rVB	117571	65874	1.76%	0.215%
29	11.848	1529	1532	1535	rBV	291713	283790	7.60%	0.927%
30	12.125	1576	1579	1586	rBV2	575576	639423	17.12%	2.089%
31	12.583	1655	1657	1660	rVB	125421	120611	3.23%	0.394%
32	12.842	1698	1701	1706	rVB	223623	221348	5.93%	0.723%
33	12.919	1711	1714	1716	rBV	193117	182704	4.89%	0.597%
34	13.072	1738	1740	1743	rBV	181974	138523	3.71%	0.453%
35	13.183	1757	1759	1760	rBV	117463	90000	2.41%	0.294%
36	13.213	1760	1764	1767	rVB	3024020	2616046	70.03%	8.546%

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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-BF013123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.107	1914	1916	1929	rVB3	251040	534996	14.32%	1.748%
38	14.277	1942	1945	1948	rBV	945667	876255	23.46%	2.863%
39	15.160	2092	2095	2101	rVB	292166	324201	8.68%	1.059%
40	15.389	2131	2134	2137	rBV2	86599	111569	2.99%	0.364%
41	15.866	2211	2215	2220	rBV2	575476	718129	19.22%	2.346%

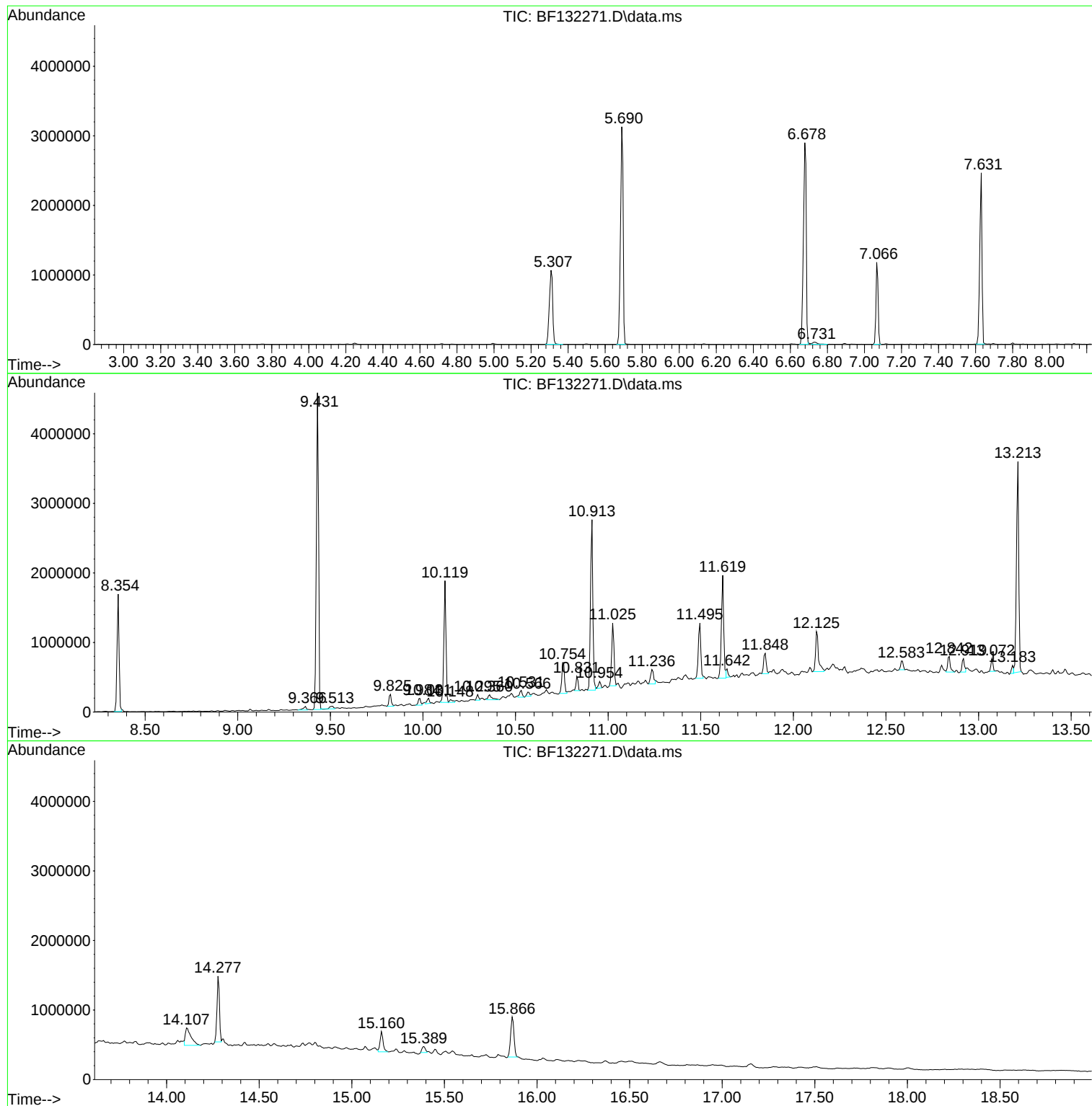
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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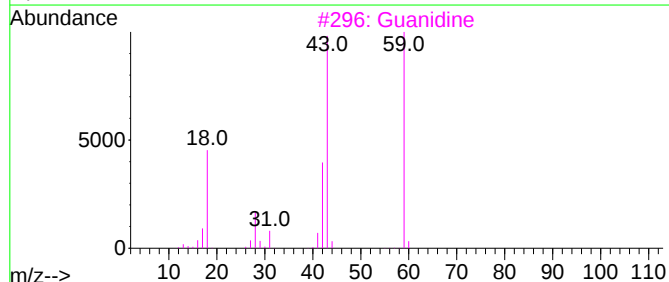
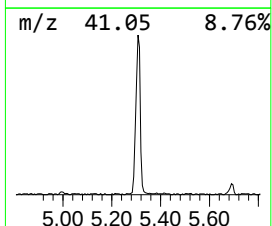
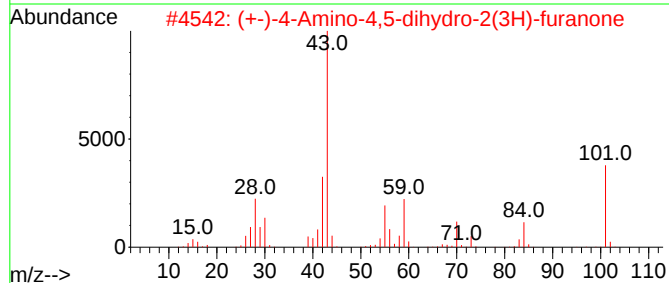
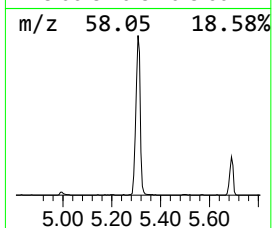
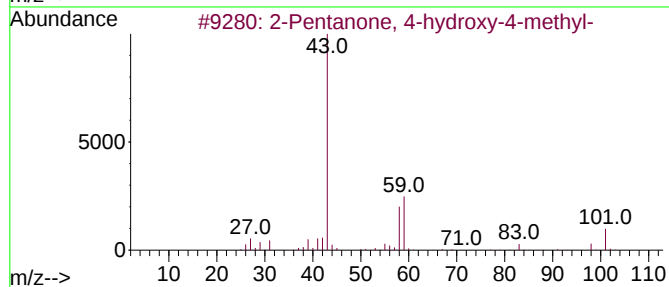
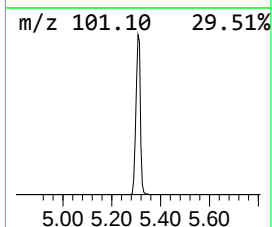
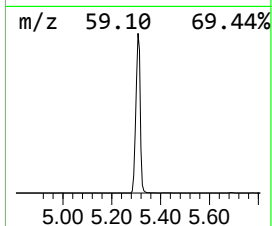
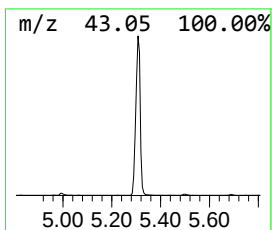
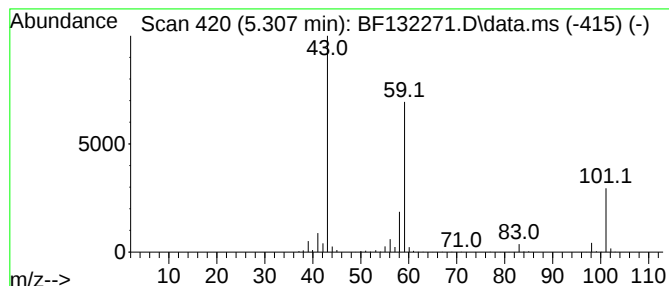
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.307	27.47 ng	1309320	1,4-Dichlorobenzene-d4	7.066

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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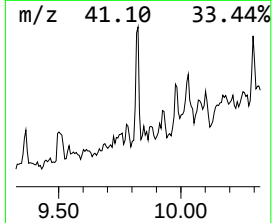
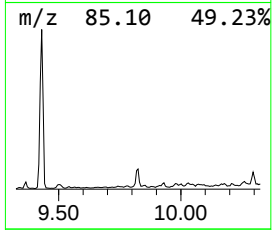
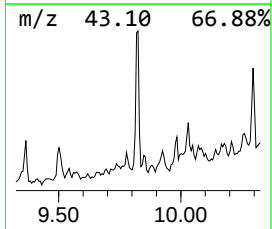
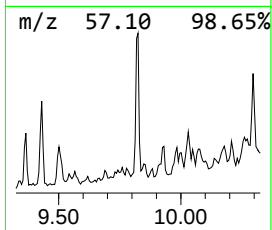
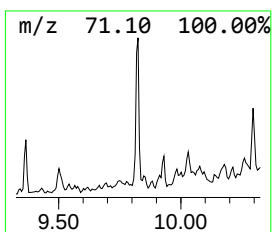
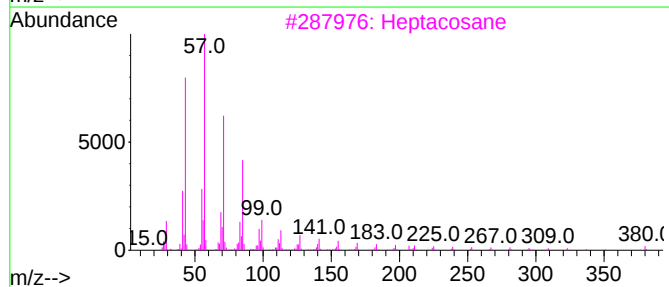
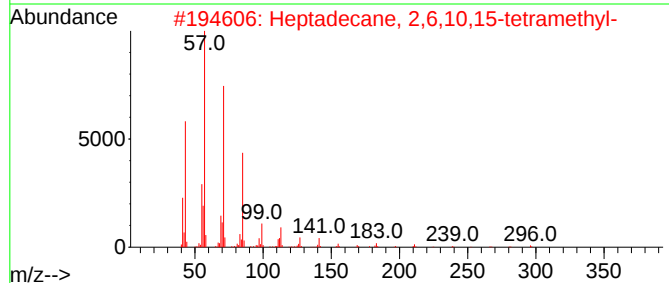
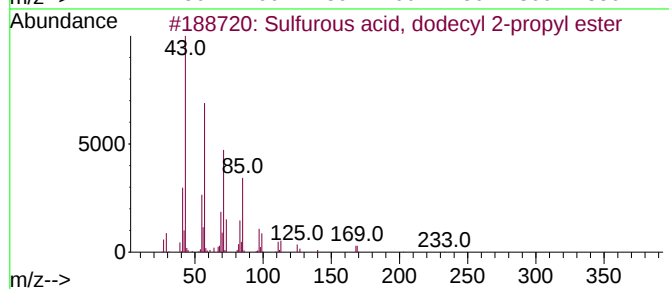
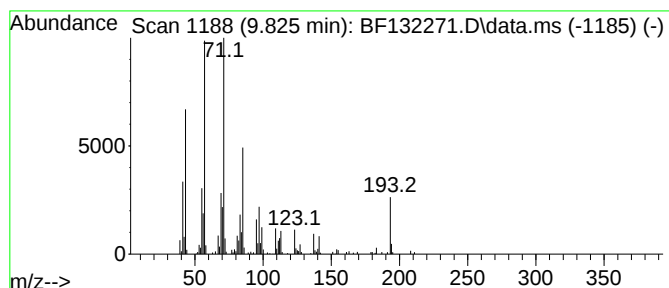
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfurous acid, dodecyl 2-p... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.825	2.29 ng	155667	Acenaphthene-d10	10.119

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	59
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	52
3			Heptacosane	380	C27H56	000593-49-7	50
4			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	50
5			Tetratetracontane	619	C44H90	007098-22-8	43



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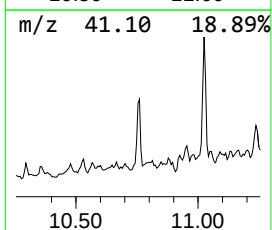
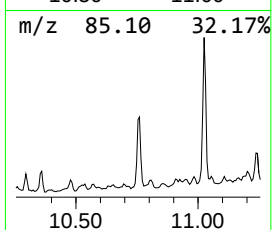
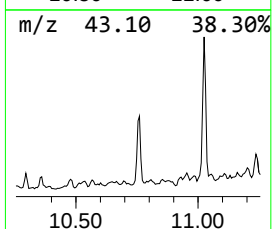
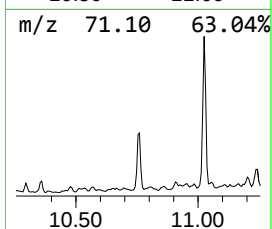
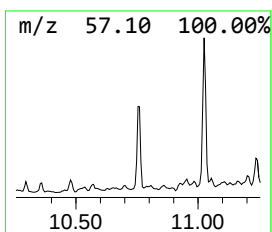
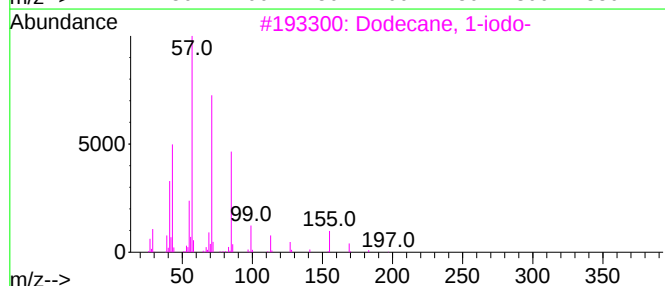
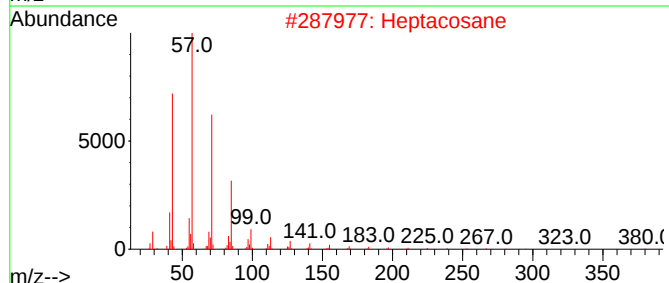
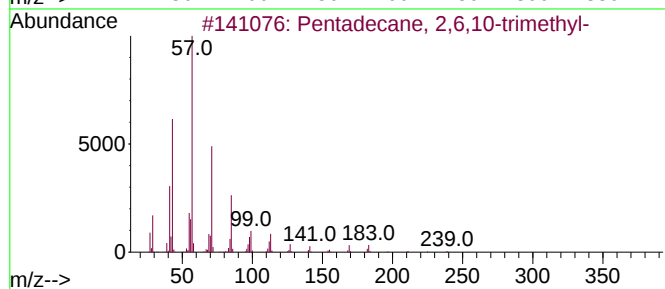
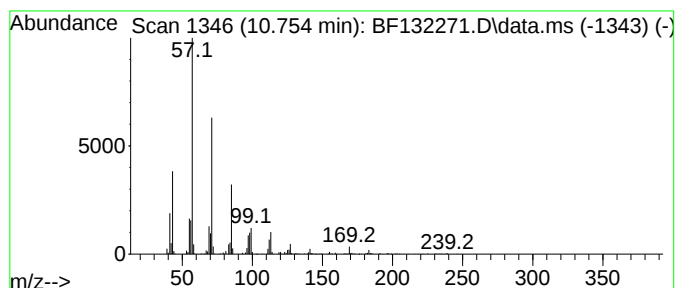
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecane, 2,6,10-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.754	6.70 ng	454773	Acenaphthene-d10	10.119	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2	Heptacosane	380	C27H56	000593-49-7	83
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	83
4	Heneicosane	296	C21H44	000629-94-7	80
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80



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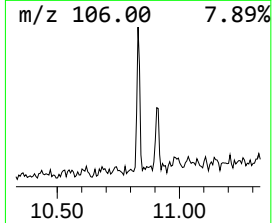
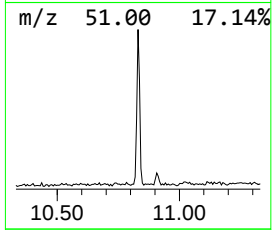
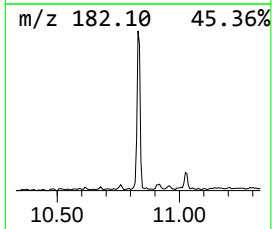
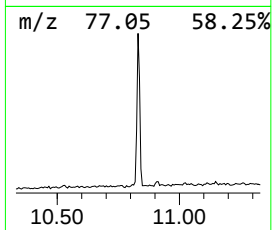
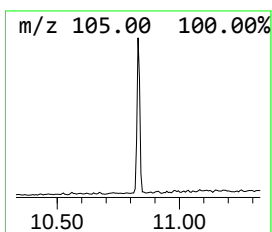
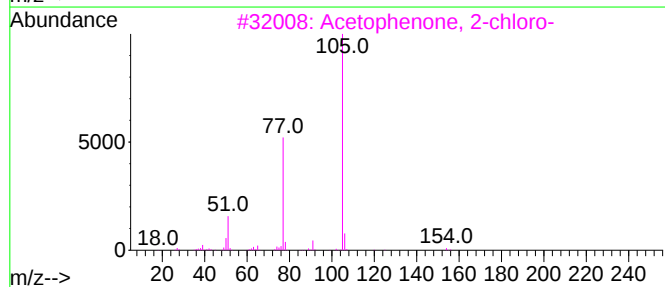
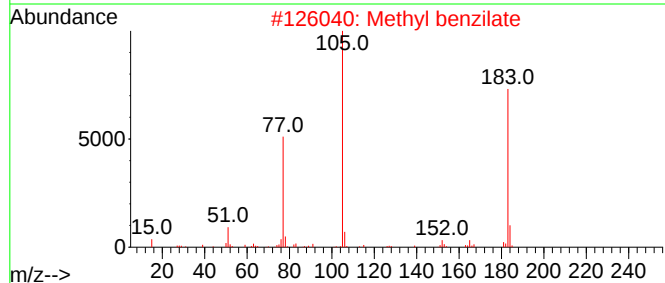
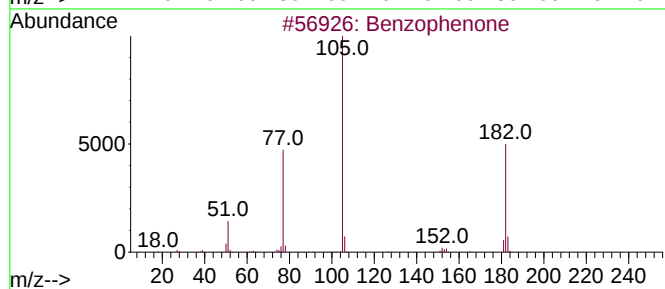
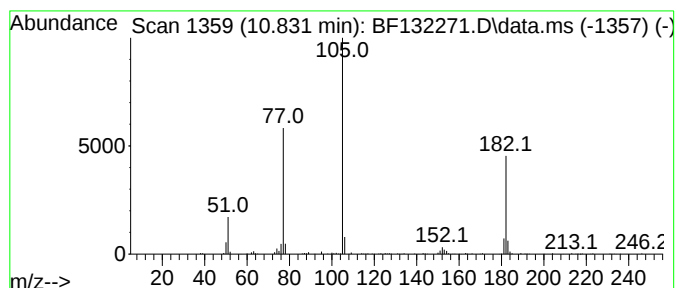
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzophenone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.831	2.23 ng	151335	Acenaphthene-d10		10.119	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzophenone		182	C13H10O	000119-61-9	94
2	Methyl benzoate		242	C15H14O3	000076-89-1	50
3	Acetophenone, 2-chloro-		154	C8H7ClO	000532-27-4	49
4	Isonitrosoacetophenone		149	C8H7NO2	000532-54-7	47
5	Methyl 2-benzoyl-4-cyanobutanoate		231	C13H13NO3	1010486-83-8	47



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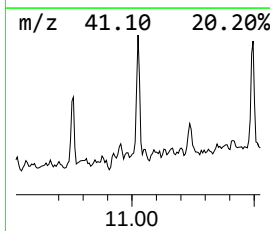
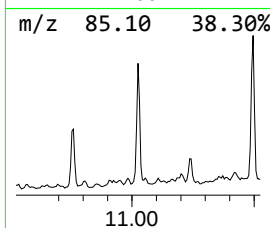
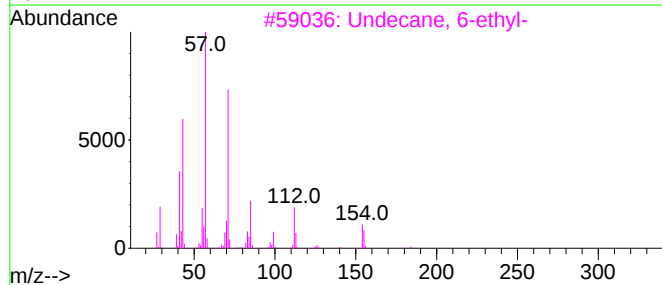
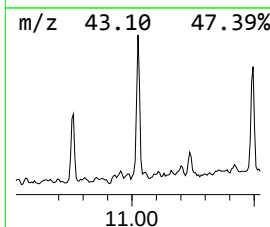
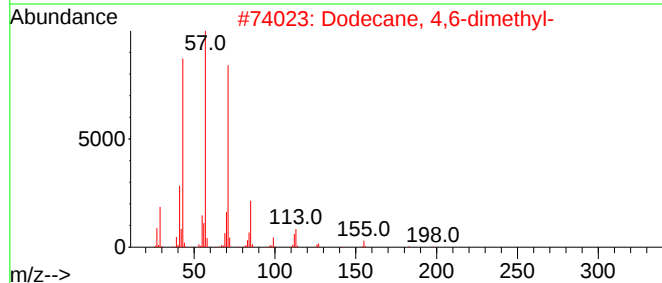
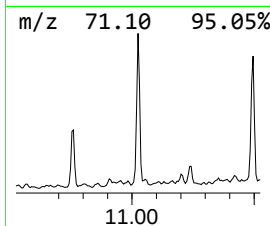
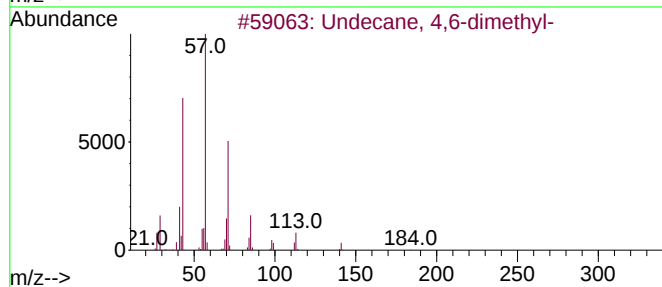
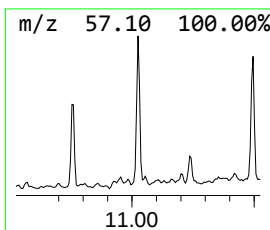
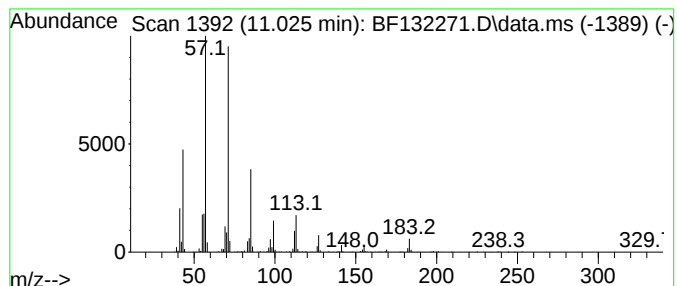
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Undecane, 4,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.025	11.96 ng	776826	Phenanthrene-d10	11.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	86
2			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	72
3			Undecane, 6-ethyl-	184	C13H28	017312-60-6	64
4			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	64
5			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
Data File : BF132271.D
Acq On : 01 Feb 2023 21:07
Operator : CG\JU
Sample : 01357-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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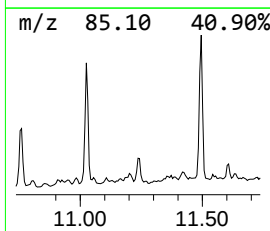
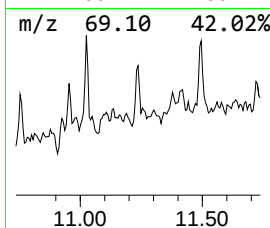
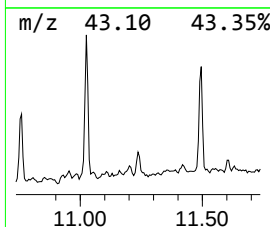
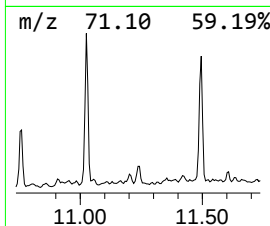
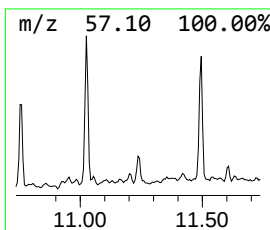
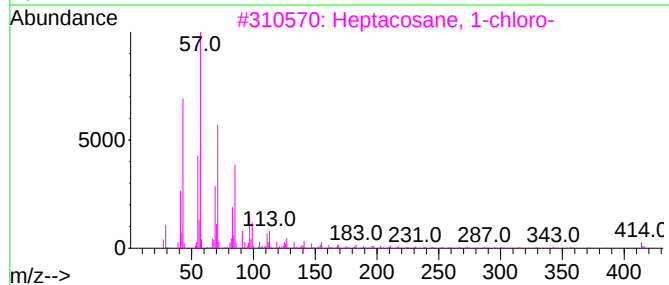
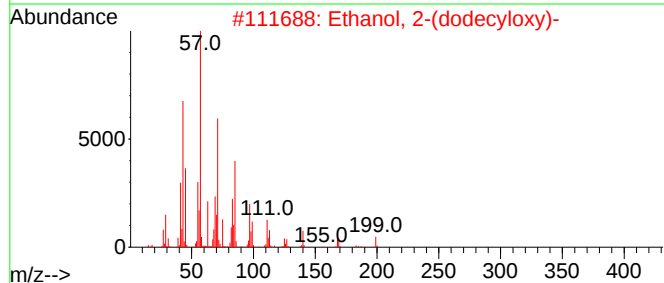
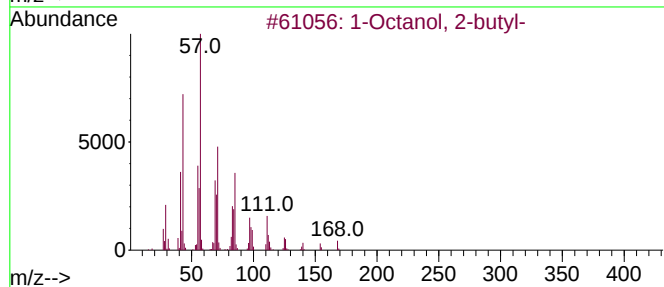
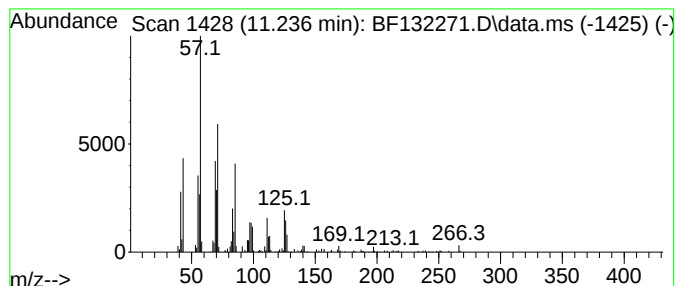
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Octanol, 2-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.236	3.70 ng	240128	Phenanthrene-d10	11.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	72
2		Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	72
3		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	64
4		Tetratetracontane	619	C44H90	007098-22-8	59
5		Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
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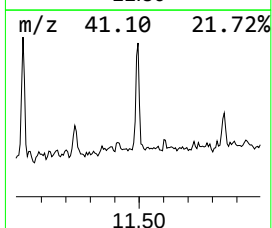
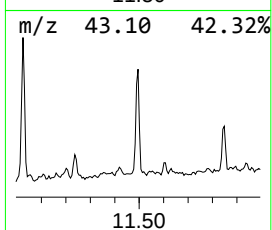
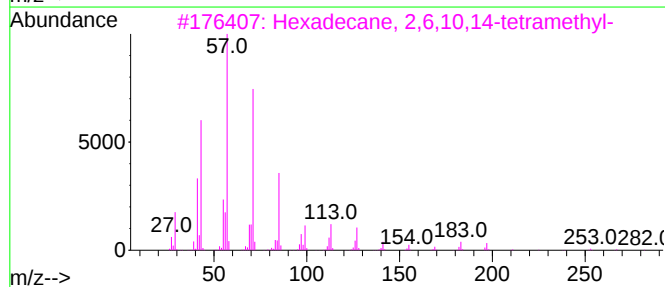
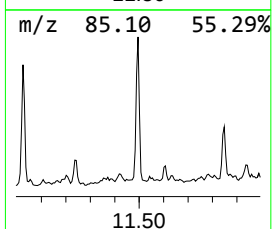
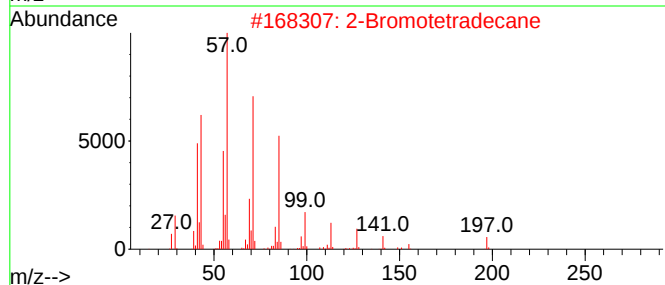
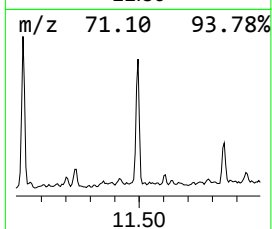
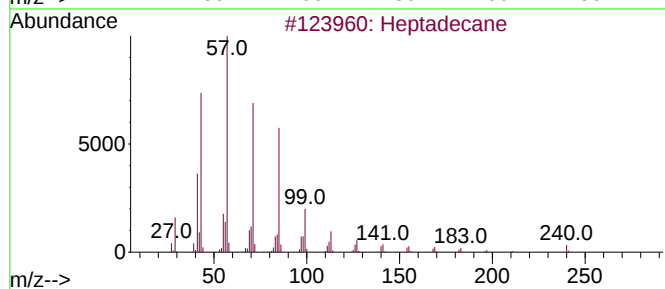
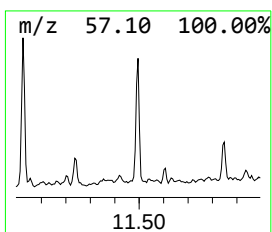
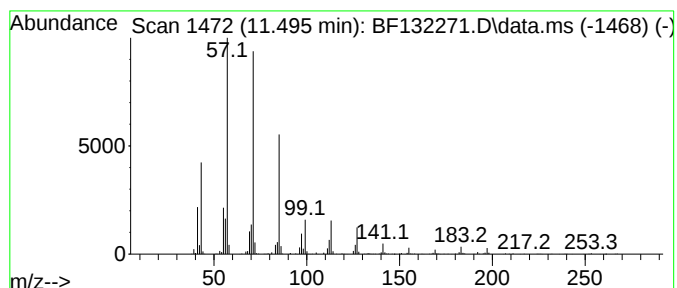
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.495	11.46 ng	744343	Phenanthrene-d10	11.619	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
4	Octadecane	254	C18H38	000593-45-3	78
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
Data File : BF132271.D
Acq On : 01 Feb 2023 21:07
Operator : CG\JU
Sample : 01357-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
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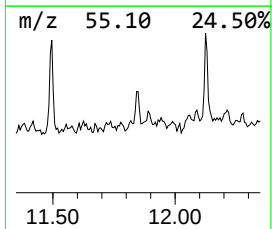
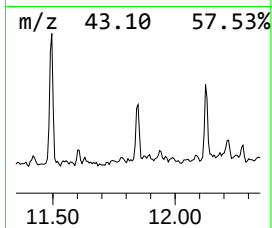
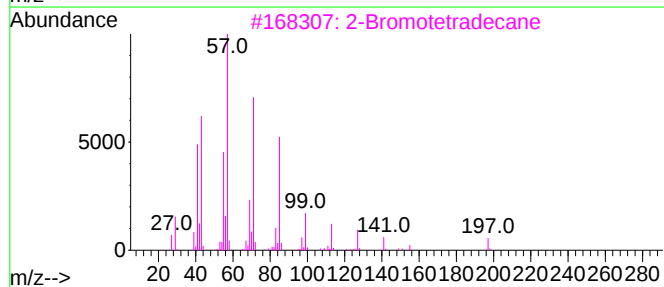
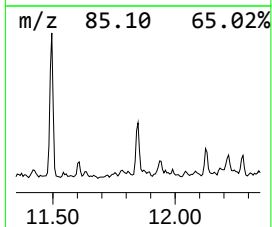
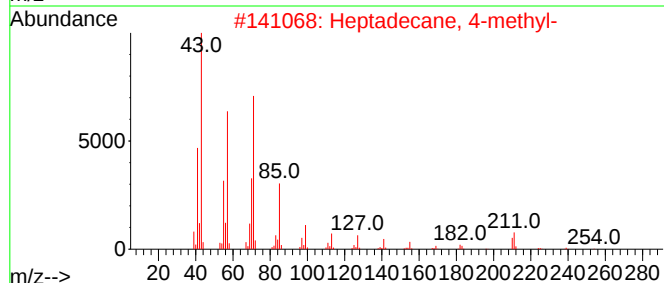
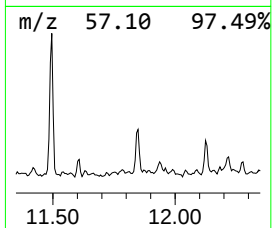
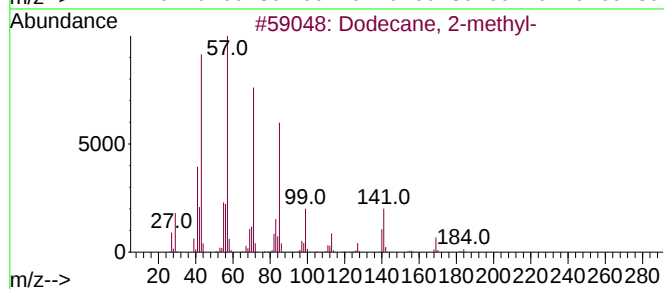
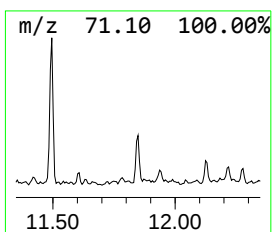
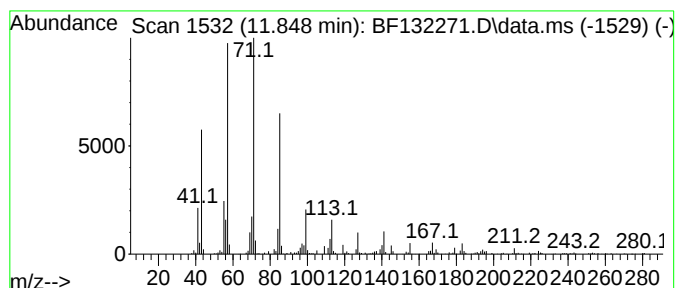
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Dodecane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.848	4.37 ng	283790	Phenanthrene-d10	11.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
2			Heptadecane, 4-methyl-	254	C18H38	026429-11-8	90
3			2-Bromotetradecane	276	C14H29Br	074036-95-6	86
4			Octadecane	254	C18H38	000593-45-3	80
5			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
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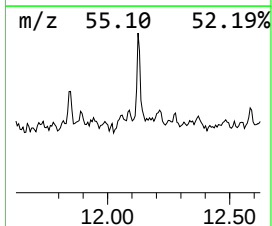
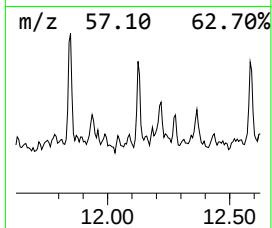
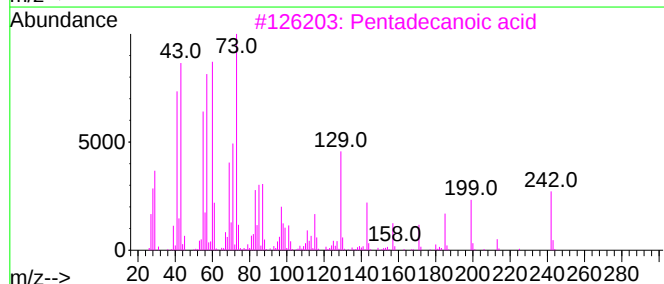
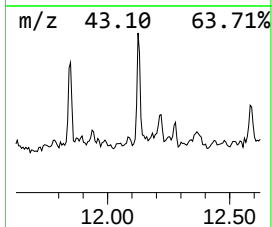
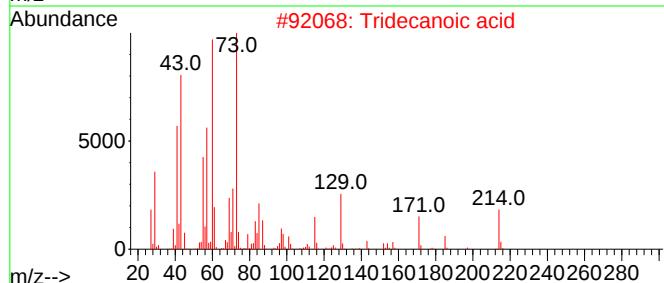
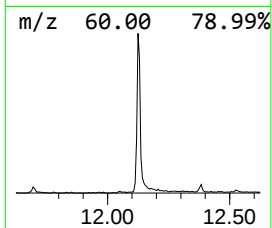
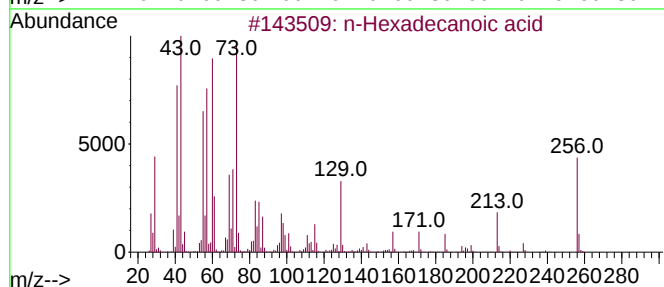
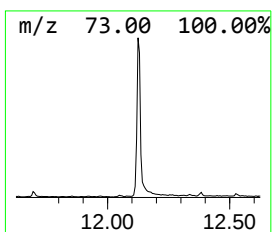
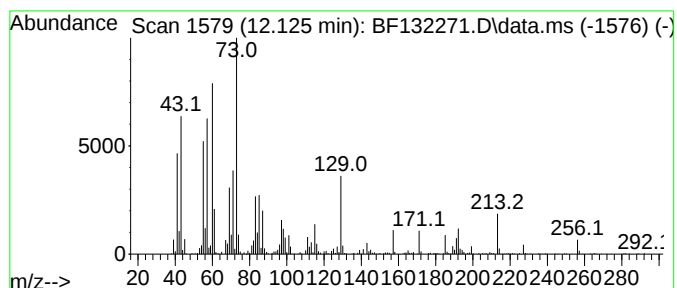
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.125	9.85 ng	639423	Phenanthrene-d10	11.619	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
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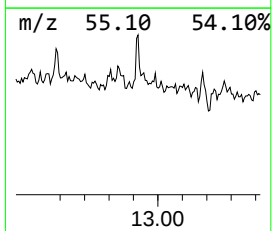
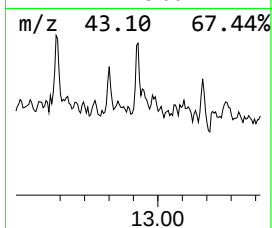
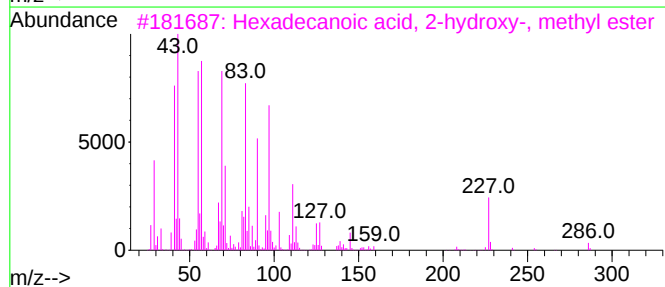
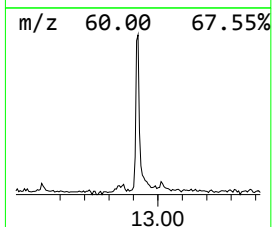
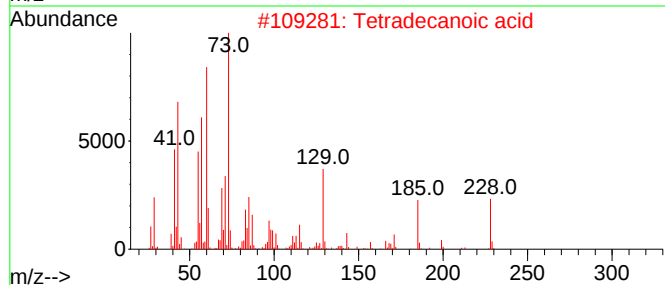
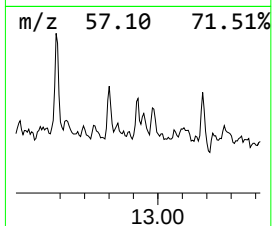
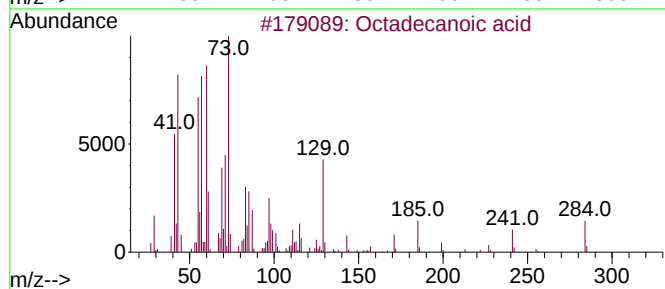
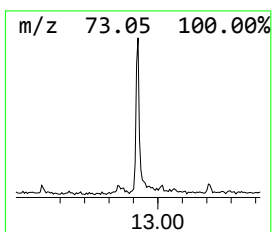
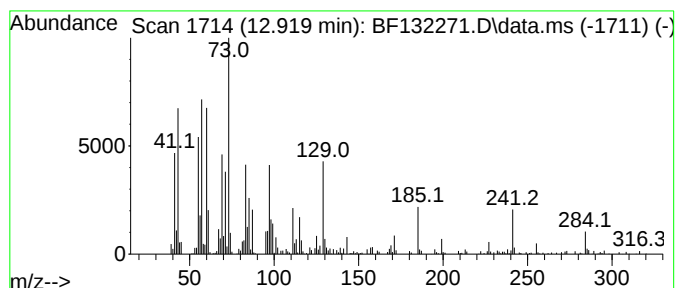
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.919	2.81 ng	182704	Phenanthrene-d10	11.619	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	55
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	Docosyl propyl ether	368	C25H52O	1000406-28-2	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
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ALS Vial : 11 Sample Multiplier: 1

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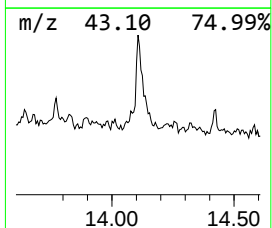
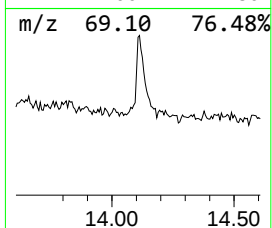
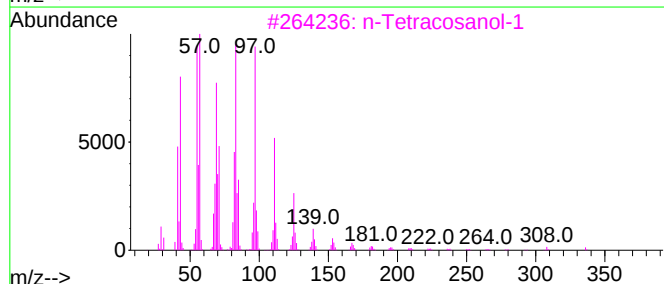
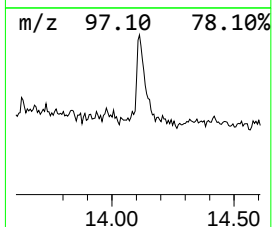
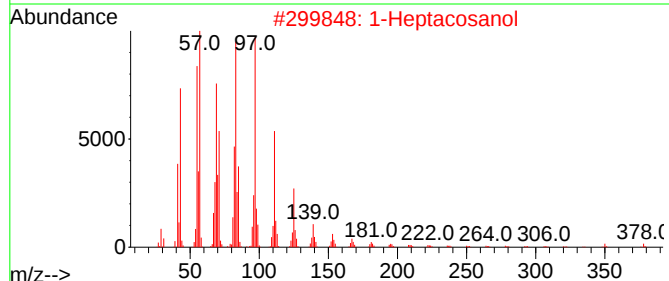
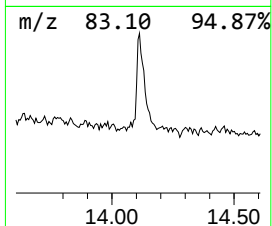
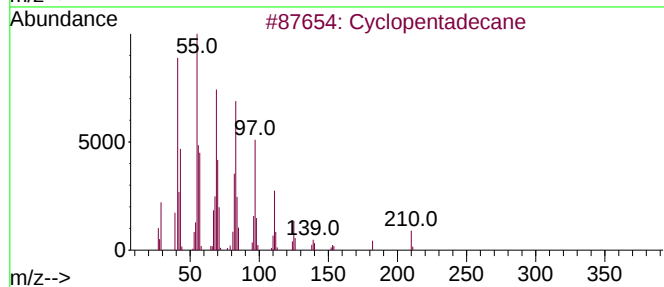
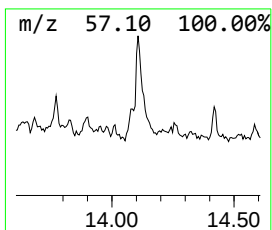
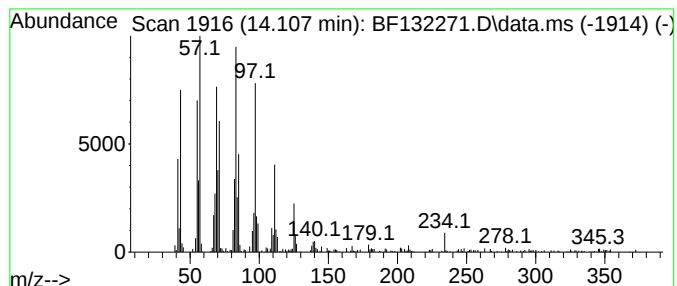
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.107	12.21 ng	534996	Chrysene-d12	14.278

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	94
2			1-Heptacosanol	396	C27H56O	002004-39-9	93
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4			17-Pentatriacontene	491	C35H70	006971-40-0	91
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
Data File : BF132271.D
Acq On : 01 Feb 2023 21:07
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
VNJ-205

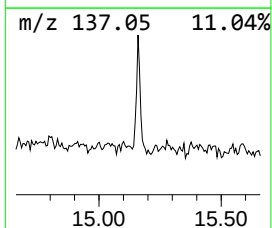
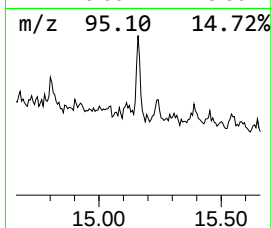
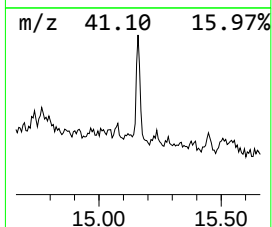
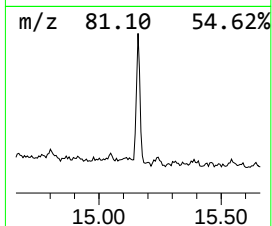
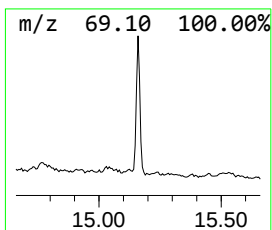
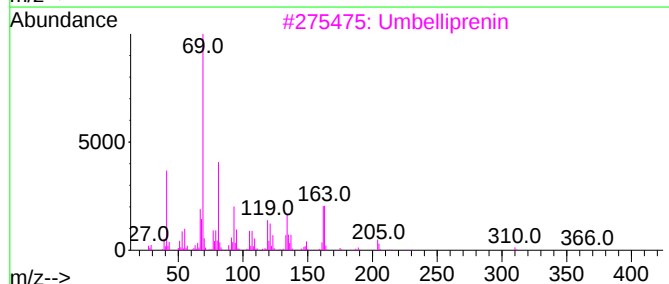
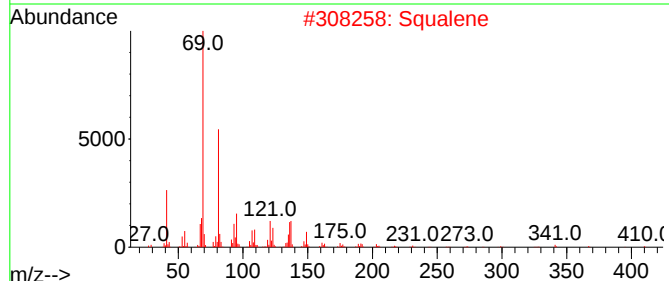
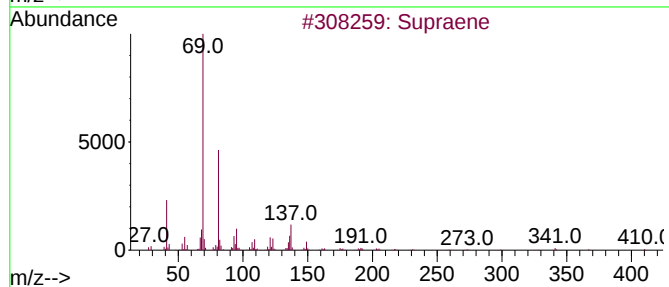
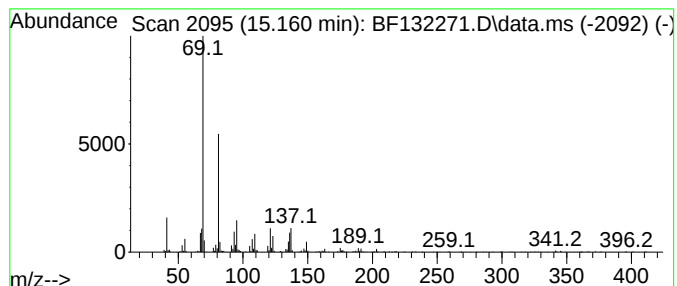
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.160	9.03 ng	324201	Perylene-d12	15.866

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	87
3			Umbelliprenin	366	C24H30O3	023838-17-7	80
4			.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
Data File : BF132271.D
Acq On : 01 Feb 2023 21:07
Operator : CG\JU
Sample : 01357-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-205

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.307	27.5	ng	1309320	1	7.066	953252	20.0
Sulfurous acid,...	9.825	2.3	ng	155667	3	10.119	1357780	20.0
Pentadecane, 2,...	10.754	6.7	ng	454773	3	10.119	1357780	20.0
Benzophenone	10.831	2.2	ng	151335	3	10.119	1357780	20.0
Undecane, 4,6-d...	11.025	12.0	ng	776826	4	11.619	1298540	20.0
1-Octanol, 2-bu...	11.236	3.7	ng	240128	4	11.619	1298540	20.0
Heptadecane	11.495	11.5	ng	744343	4	11.619	1298540	20.0
Dodecane, 2-met...	11.848	4.4	ng	283790	4	11.619	1298540	20.0
n-Hexadecanoic ...	12.125	9.8	ng	639423	4	11.619	1298540	20.0
Octadecanoic acid	12.919	2.8	ng	182704	4	11.619	1298540	20.0
Cyclopentadecane	14.107	12.2	ng	534996	5	14.278	876255	20.0
Supraene	15.160	9.0	ng	324201	6	15.866	718129	20.0