

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051325\
 Data File : BF142339.D
 Acq On : 13 May 2025 12:19
 Operator : RC/JU
 Sample : Q1985-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW8-BW-20250507

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-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142339.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.116	488	497	504	rBV	170479	251884	3.69%	0.668%
2	5.510	558	564	570	rBV	2085421	2801380	41.02%	7.425%
3	6.516	729	735	740	rBV	1428364	1807160	26.46%	4.790%
4	6.904	796	801	806	rBV	1005639	1228795	17.99%	3.257%
5	7.463	889	896	901	rBV	2801520	3847710	56.35%	10.199%
6	8.187	1013	1019	1024	rBV	1267497	1619645	23.72%	4.293%
7	9.263	1195	1202	1207	rBV	5163499	6828712	100.00%	18.100%
8	9.939	1311	1317	1322	rBV	1477190	1823452	26.70%	4.833%
9	10.651	1433	1438	1445	rVB	198887	264788	3.88%	0.702%
10	10.728	1445	1451	1456	rBV	3345563	4405050	64.51%	11.676%
11	11.428	1565	1570	1575	rVB	1418940	1762580	25.81%	4.672%
12	11.845	1632	1641	1651	rBV3	23508	77225	1.13%	0.205%
13	11.945	1652	1658	1662	rBV	160325	267628	3.92%	0.709%
14	11.986	1662	1665	1675	rVB	302732	390104	5.71%	1.034%
15	12.698	1781	1786	1788	rBV	80137	104891	1.54%	0.278%
16	12.733	1788	1792	1805	rVB	118762	239100	3.50%	0.634%
17	13.016	1834	1840	1845	rBV	4676854	6202575	90.83%	16.441%
18	13.404	1900	1906	1912	rBV	47554	85368	1.25%	0.226%
19	13.586	1928	1937	1945	rVB	64031	115772	1.70%	0.307%
20	13.916	1987	1993	1996	rBV	111608	163992	2.40%	0.435%
21	13.951	1996	1999	2007	rVV	52764	102207	1.50%	0.271%
22	14.063	2011	2018	2025	rBV	866552	1258288	18.43%	3.335%
23	14.227	2041	2046	2056	rVB	128287	192764	2.82%	0.511%
24	14.427	2076	2080	2088	rBV	59534	102850	1.51%	0.273%
25	14.533	2094	2098	2105	rVB	134471	186403	2.73%	0.494%
26	14.851	2147	2152	2155	rBV	113319	172496	2.53%	0.457%
27	15.198	2206	2211	2223	rBV	81926	153142	2.24%	0.406%
28	15.557	2266	2272	2287	rBV	745289	1271209	18.62%	3.369%

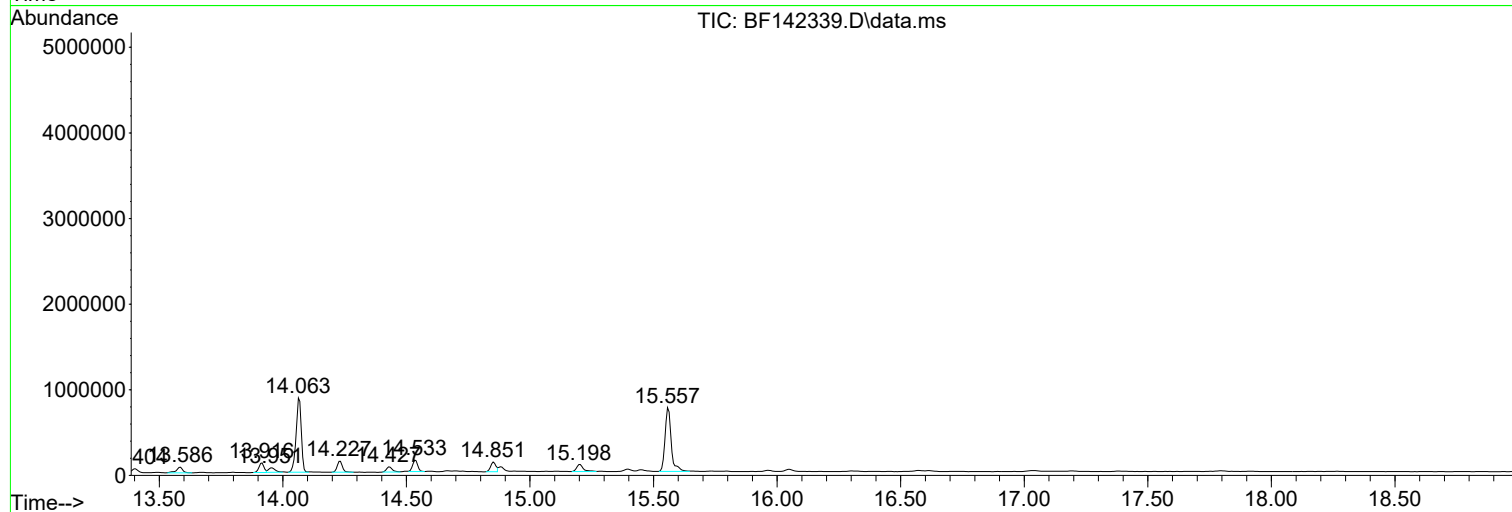
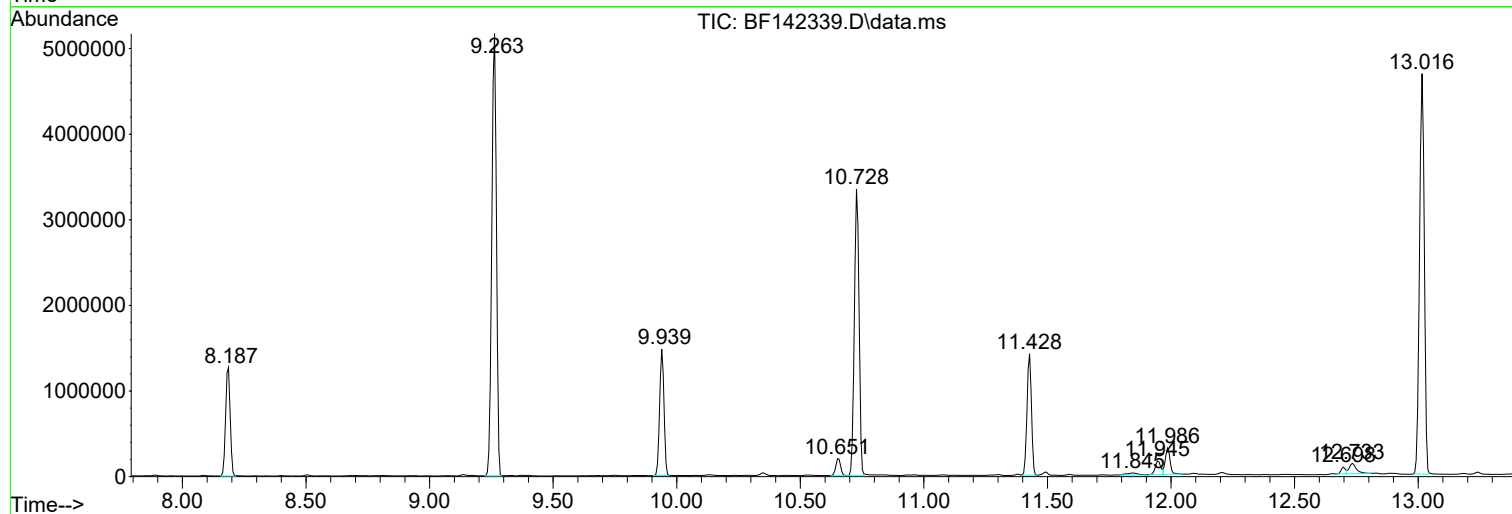
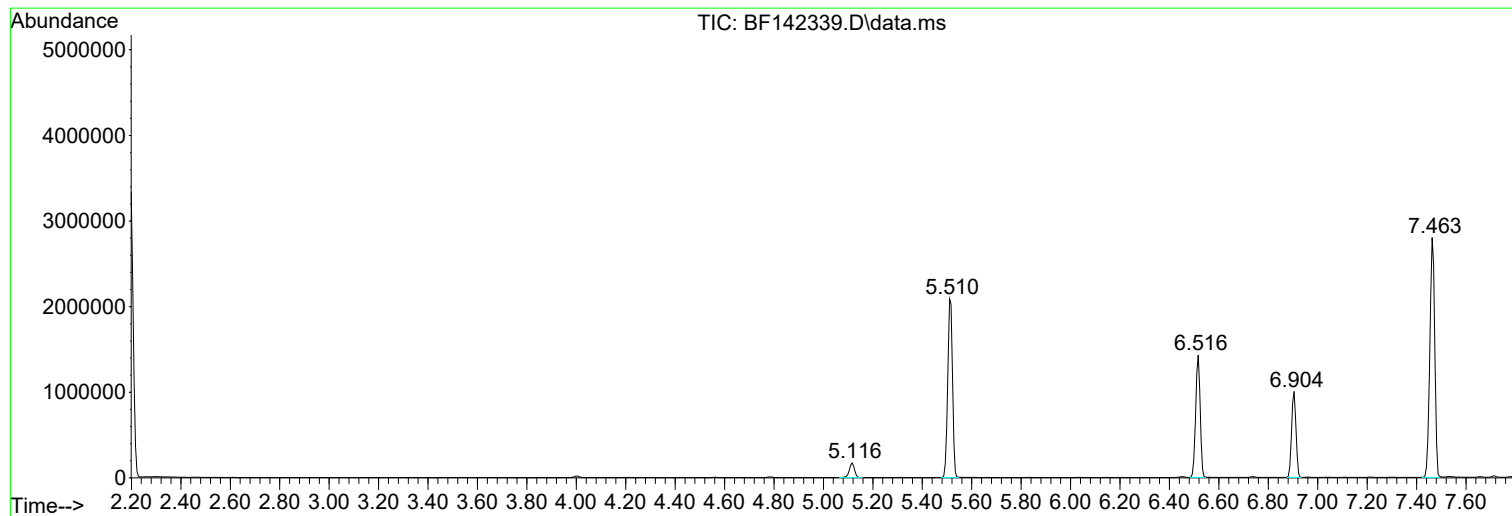
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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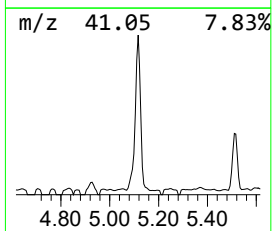
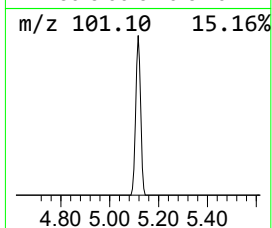
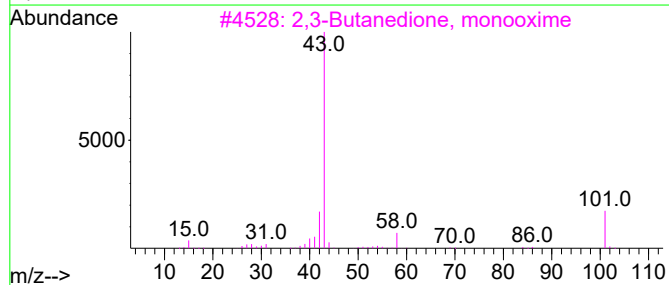
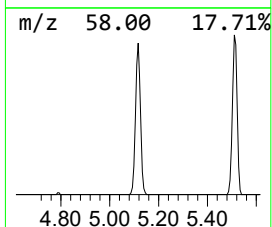
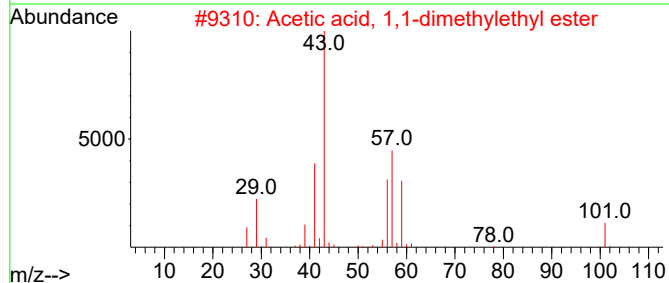
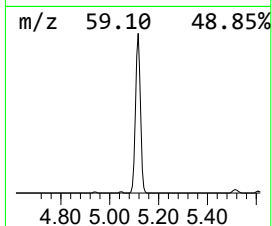
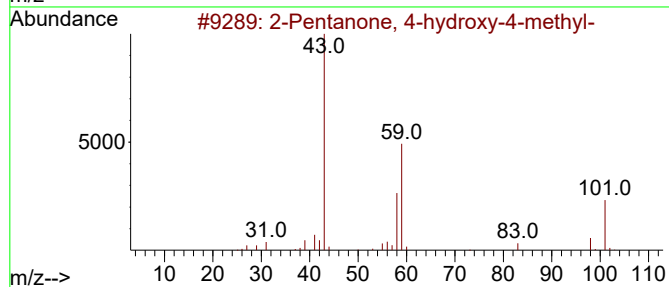
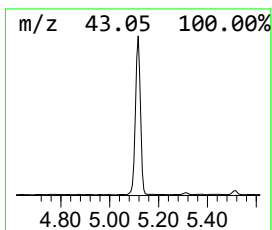
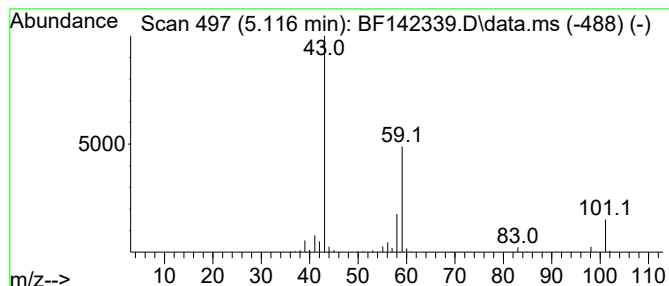
Instrument :
BNA_F
ClientSampleId :
RW8-BW-20250507

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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.	
5.116	4.10 ng	251884	1,4-Dichlorobenzene-d4		6.904	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	28
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	16
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	12
5	Acetone		58	C3H6O	000067-64-1	12



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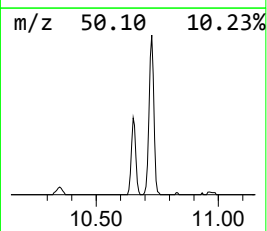
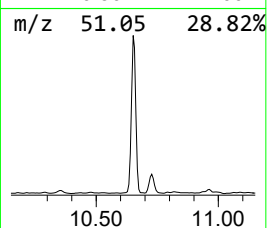
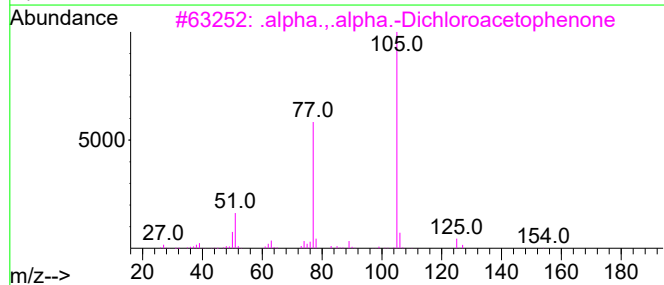
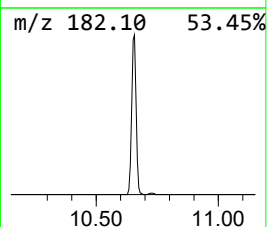
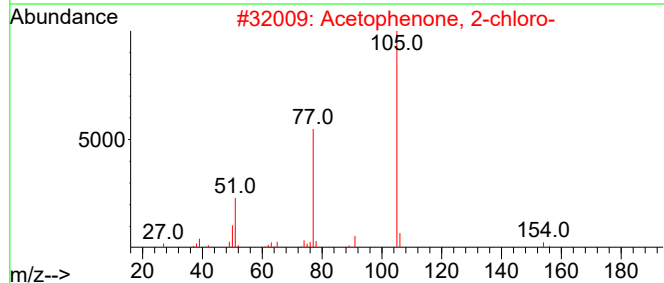
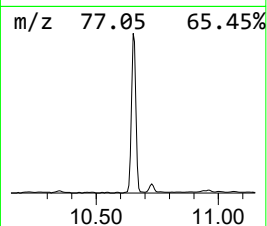
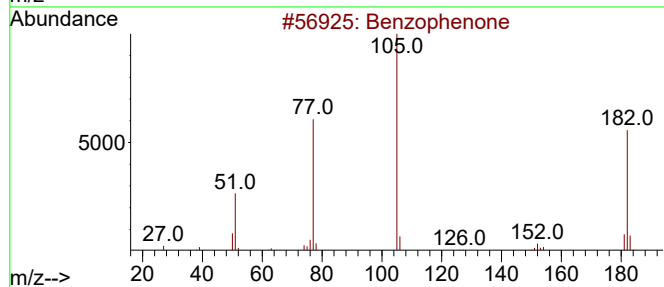
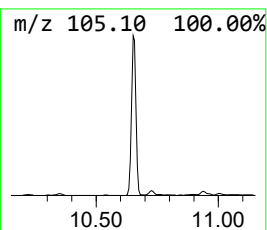
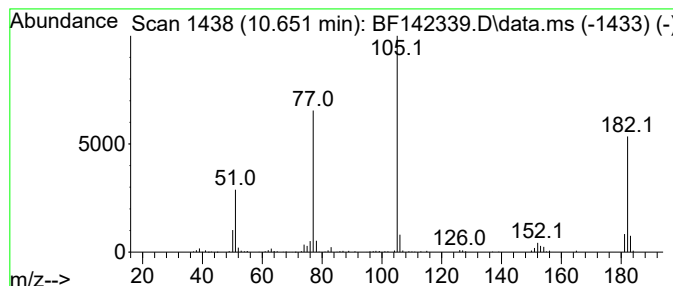
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	2.90 ng	264788	Acenaphthene-d10	9.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	52
3			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	50
4			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	50
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	50



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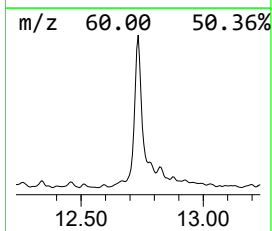
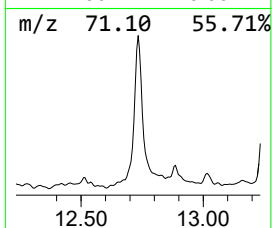
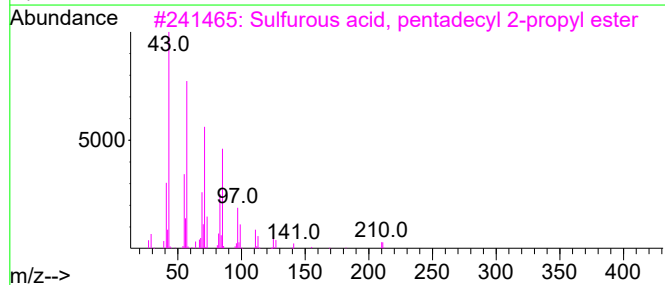
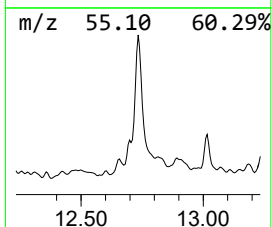
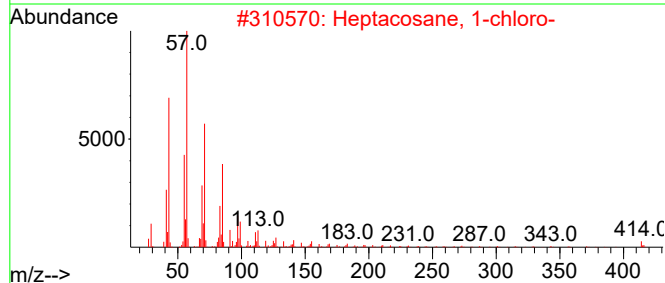
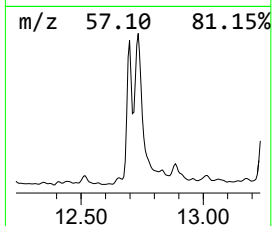
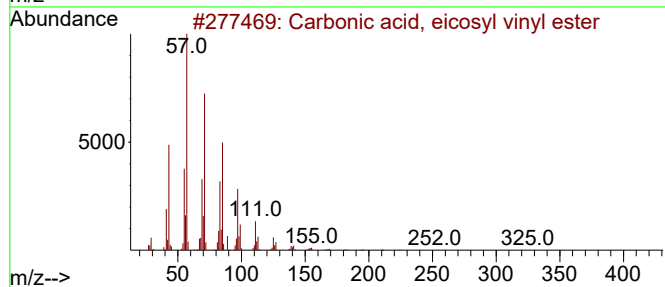
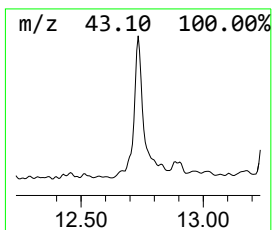
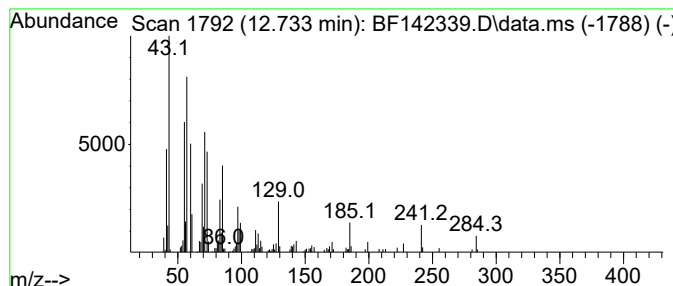
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Carbonic acid, eicosyl vinyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.733	2.71 ng	239100	Phenanthrene-d10	11.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	55
2			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	49
3			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	49
4			Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1010309-12-5	49
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	49



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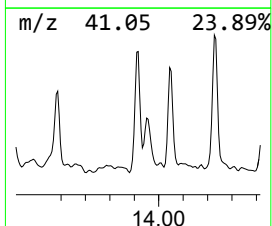
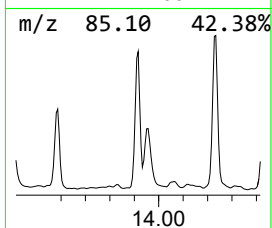
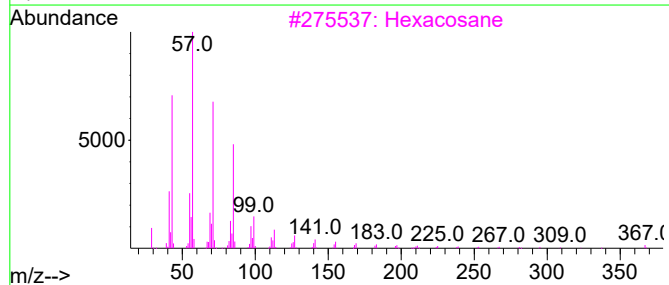
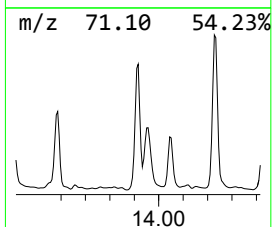
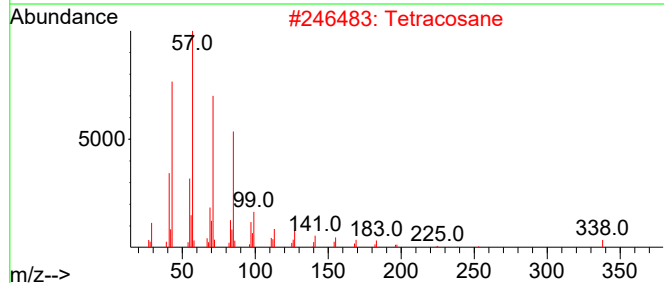
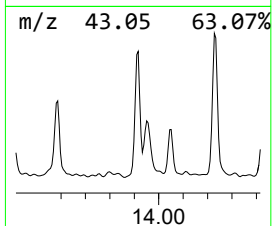
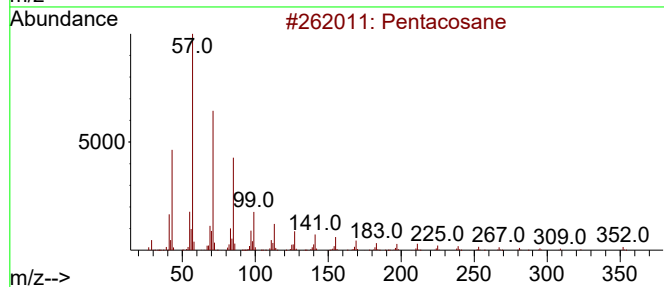
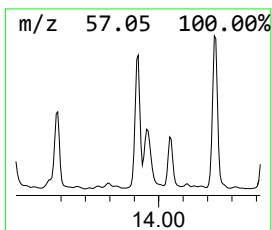
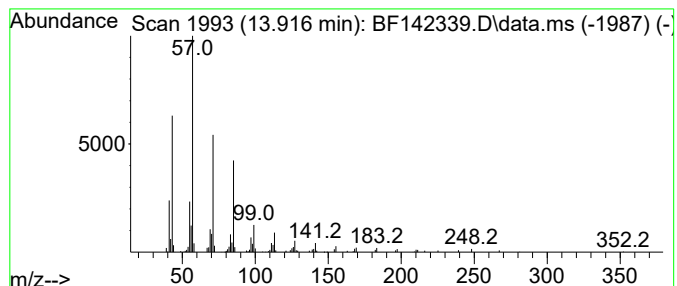
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.916	2.61 ng	163992	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	90
2			Tetracosane	338	C24H50	000646-31-1	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Octacosane	394	C28H58	000630-02-4	90



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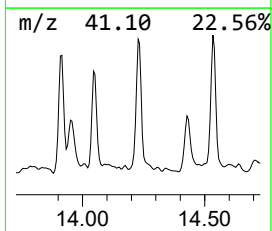
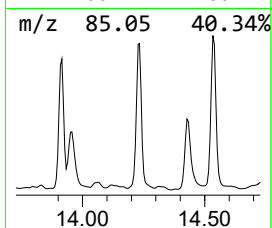
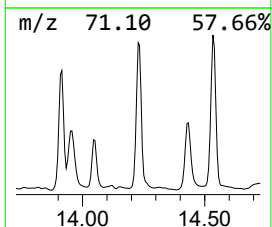
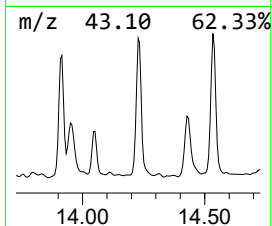
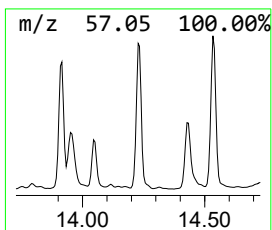
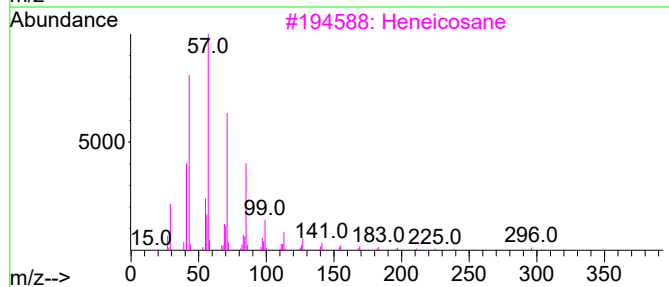
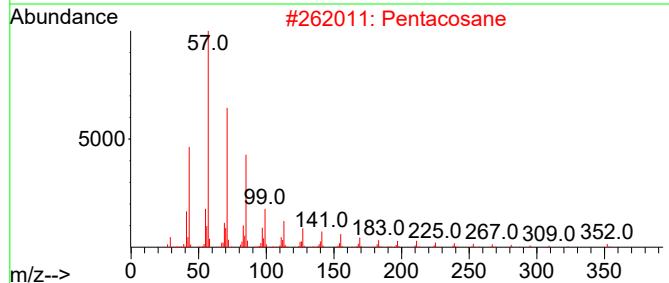
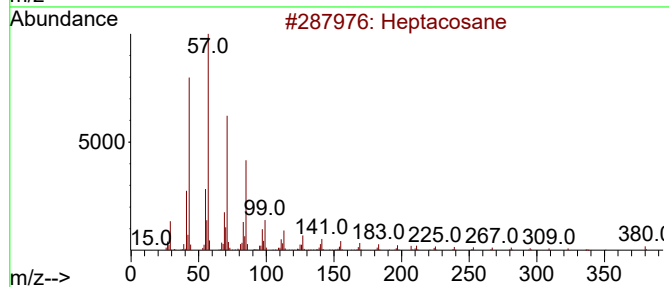
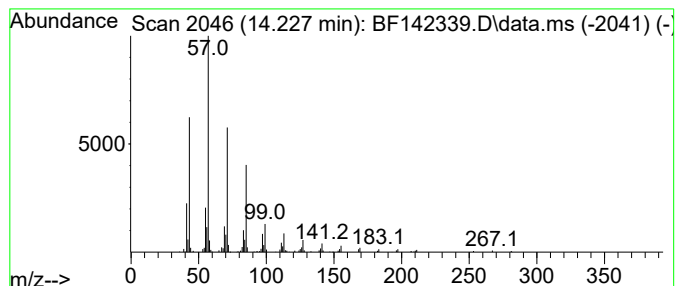
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Peak Number 5 Heptacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.227	3.06 ng	192764	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Pentacosane	352	C25H52	000629-99-2	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Eicosane	282	C20H42	000112-95-8	91
5			Hexacosane	366	C26H54	000630-01-3	91



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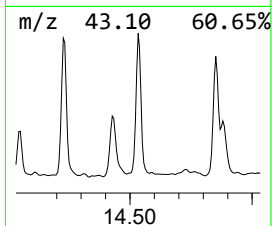
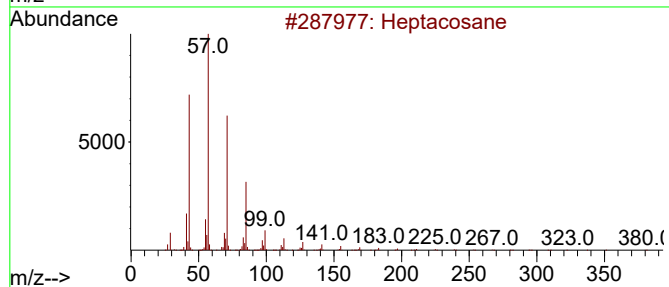
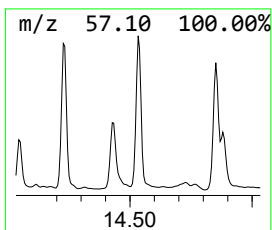
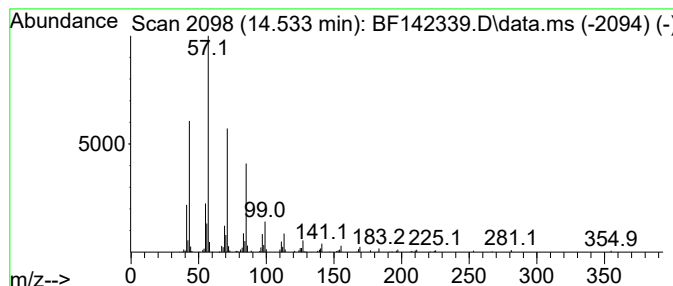
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	2.96 ng	186403	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Pentacosane	352	C25H52	000629-99-2	91
5			Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051325\
Data File : BF142339.D
Acq On : 13 May 2025 12:19
Operator : RC/JU
Sample : Q1985-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW8-BW-20250507

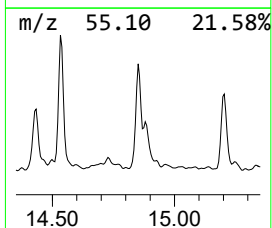
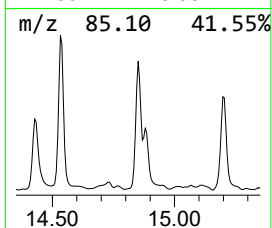
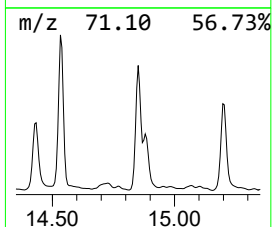
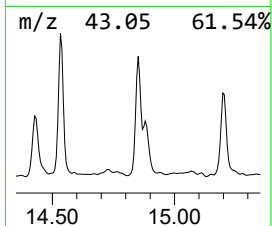
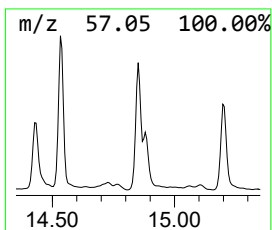
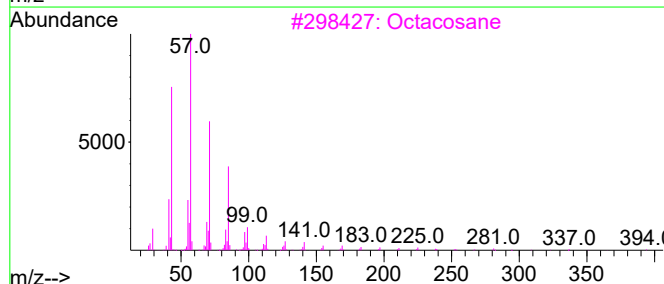
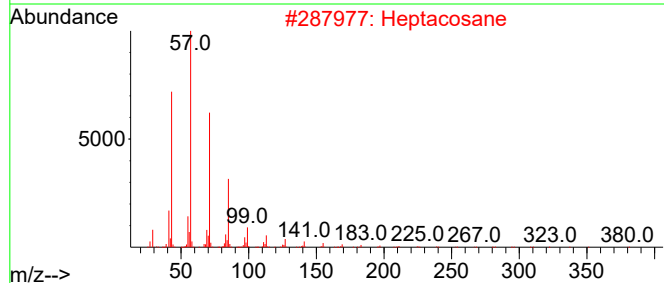
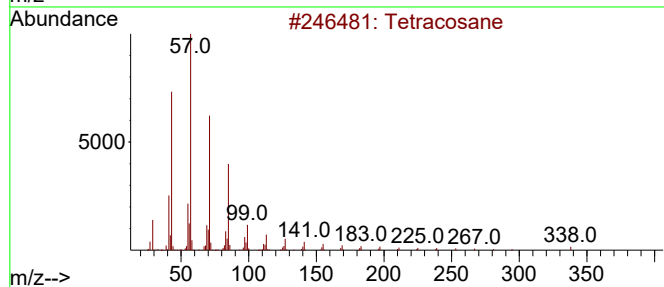
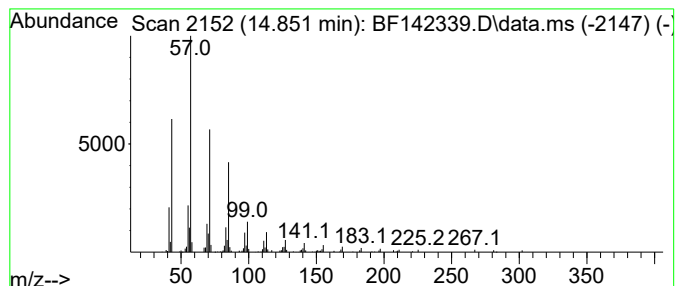
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	2.71 ng	172496	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Heptacosane	380	C27H56	000593-49-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Tetratetracontane	619	C44H90	007098-22-8	91
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051325\
Data File : BF142339.D
Acq On : 13 May 2025 12:19
Operator : RC/JU
Sample : Q1985-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW8-BW-20250507

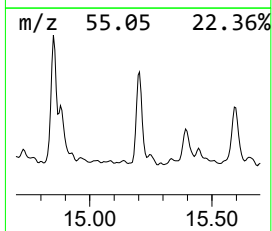
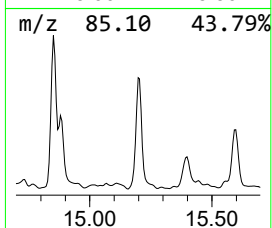
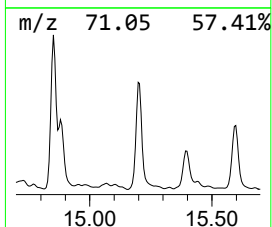
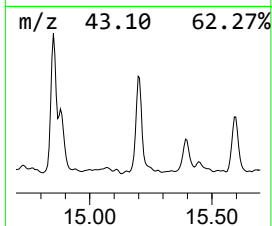
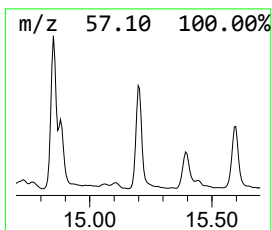
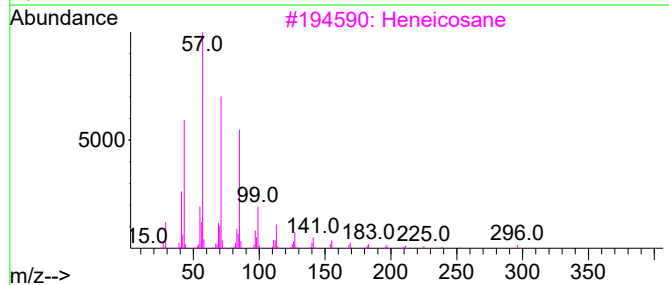
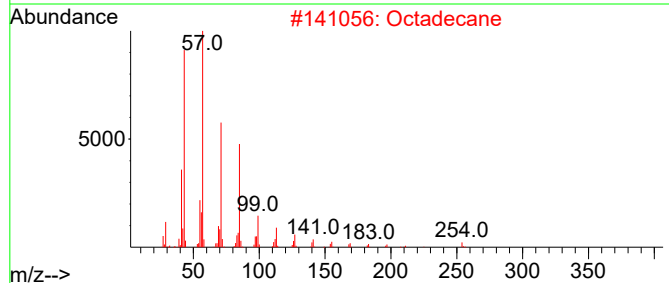
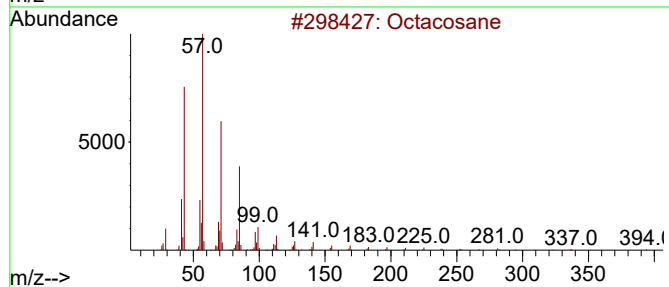
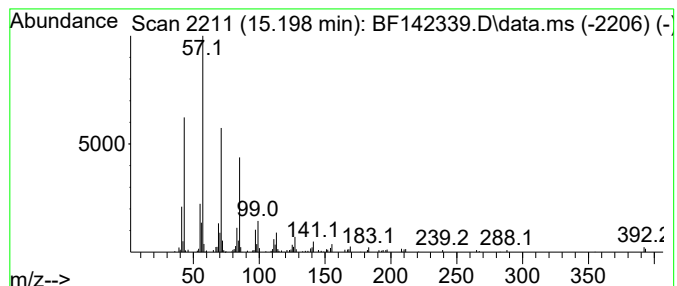
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	2.41 ng	153142	Perylene-d12	15.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Octadecane	254	C18H38	000593-45-3	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Hentriacontane	437	C31H64	000630-04-6	90
5			Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051325\
Data File : BF142339.D
Acq On : 13 May 2025 12:19
Operator : RC/JU
Sample : Q1985-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW8-BW-20250507

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.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-...	5.116	4.1	ng	251884	1	6.904	1228800	20.0
Benzophenone	10.651	2.9	ng	264788	3	9.939	1823450	20.0
Carbonic acid, ...	12.733	2.7	ng	239100	4	11.428	1762580	20.0
Pentacosane	13.916	2.6	ng	163992	5	14.063	1258290	20.0
Heptacosane	14.227	3.1	ng	192764	5	14.063	1258290	20.0
Tetracosane	14.533	3.0	ng	186403	5	14.063	1258290	20.0
Octacosane	14.851	2.7	ng	172496	6	15.557	1271210	20.0
Octadecane	15.198	2.4	ng	153142	6	15.557	1271210	20.0