

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
 Data File : BF135527.D
 Acq On : 02 Oct 2023 15:02
 Operator : CG\JU
 Sample : 04668-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR251697

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-BF091123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135527.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.369	555	558	573	rBV	2378833	2643472	100.00%	16.373%
2	6.392	729	732	750	rBV	2761628	2565595	97.05%	15.891%
3	6.745	788	792	798	rBV	894883	795649	30.10%	4.928%
4	7.310	884	888	891	rBV	1773615	1529176	57.85%	9.471%
5	8.022	1006	1009	1012	rVB	1313776	964635	36.49%	5.975%
6	8.069	1012	1017	1020	rBV6	149086	194932	7.37%	1.207%
7	8.186	1034	1037	1041	rBV3	140548	205500	7.77%	1.273%
8	8.404	1071	1074	1076	rBV3	163522	201330	7.62%	1.247%
9	14.433	2096	2099	2107	rVB	1732941	2288446	86.57%	14.174%
10	15.404	2260	2264	2270	rVB	753319	1003647	37.97%	6.216%
11	15.851	2336	2340	2346	rVB	218430	308369	11.67%	1.910%
12	16.951	2524	2527	2535	rVB2	103549	180715	6.84%	1.119%
13	17.974	2692	2701	2711	rVB3	699149	1959853	74.14%	12.139%
14	18.262	2741	2750	2761	rVB5	253051	702261	26.57%	4.350%
15	18.456	2776	2783	2799	rVB5	194709	601822	22.77%	3.728%

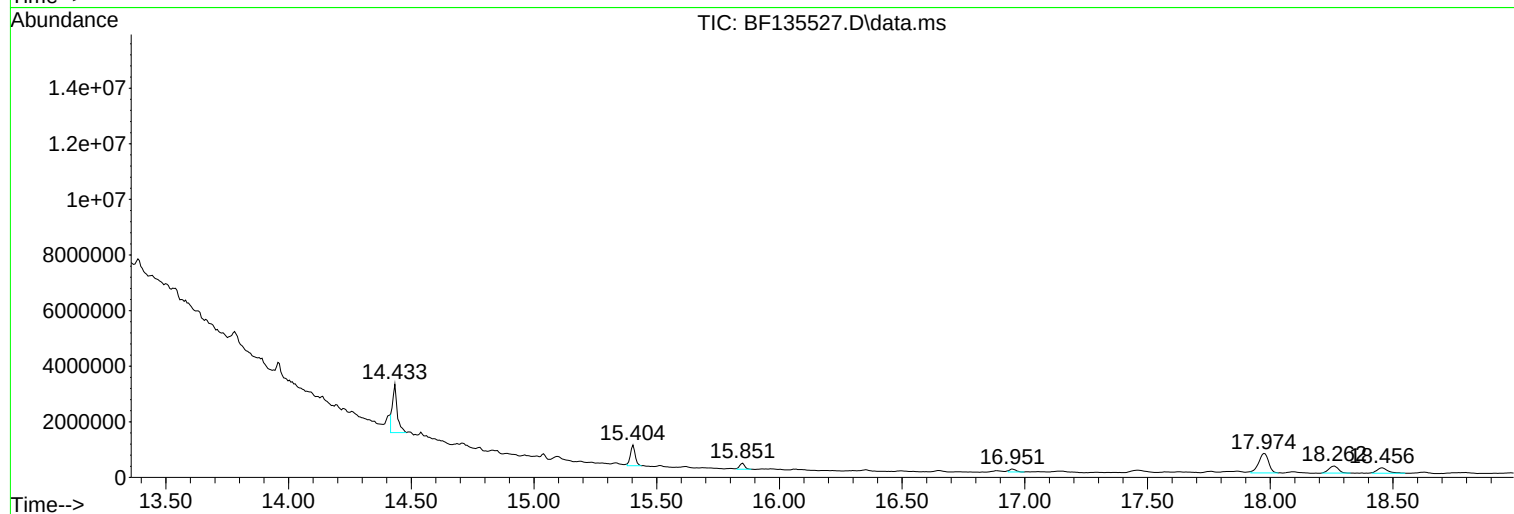
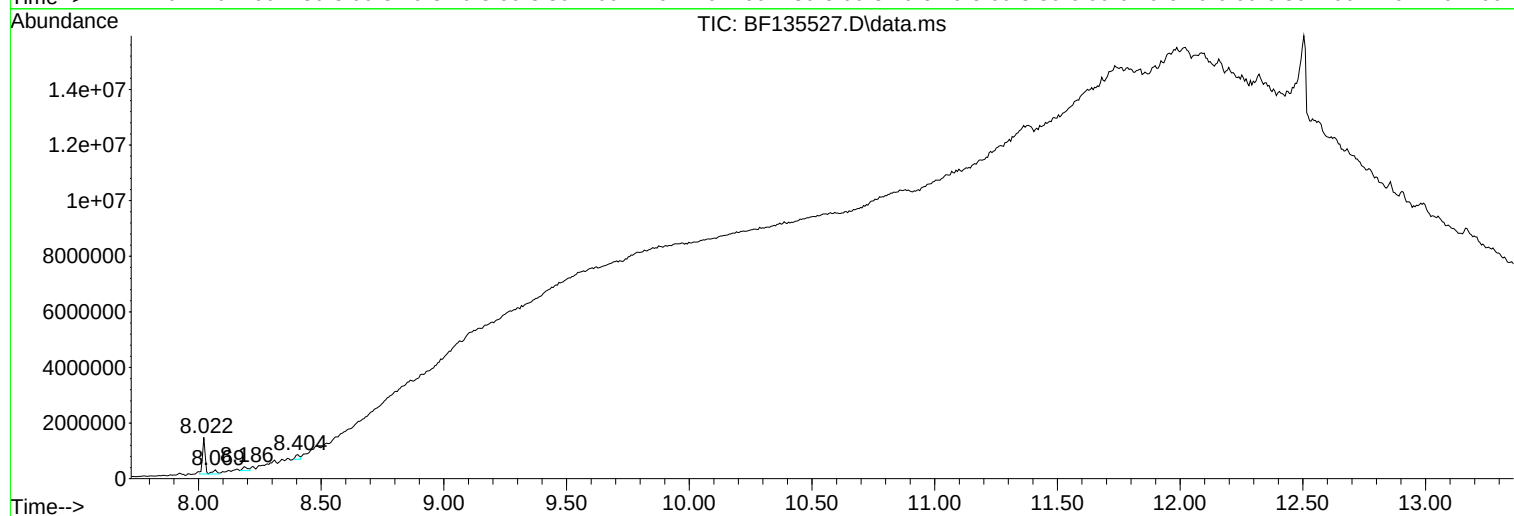
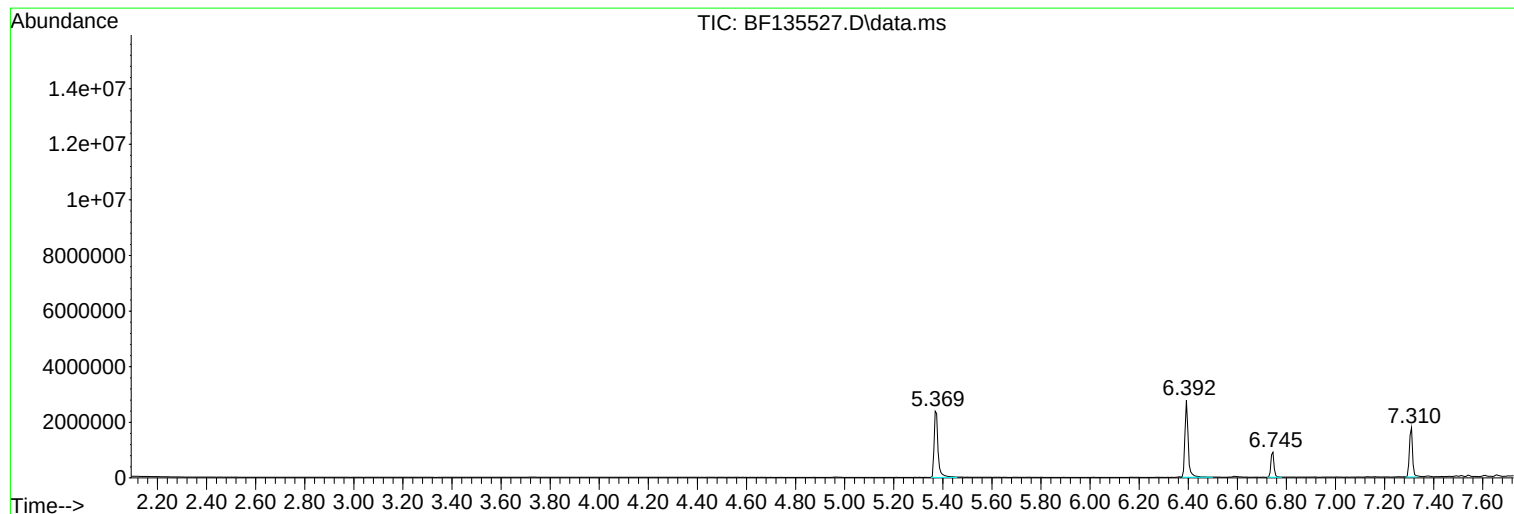
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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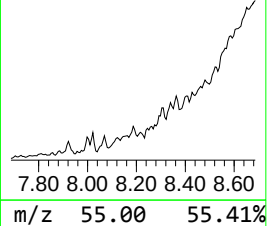
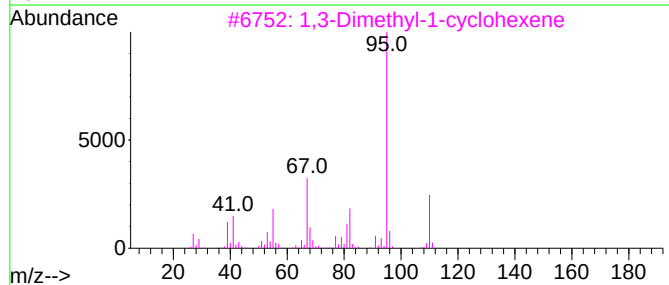
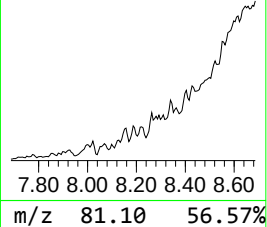
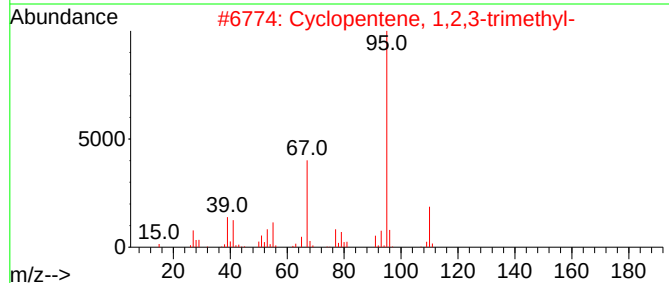
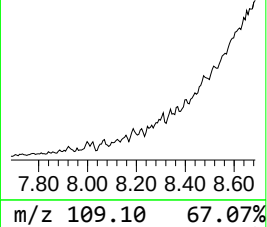
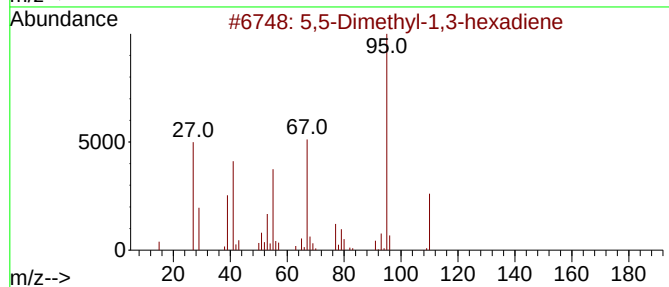
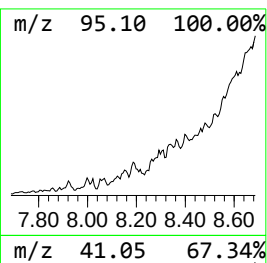
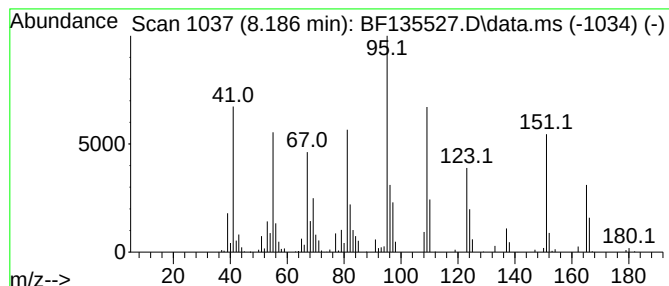
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Peak Number 1 unknown8.186 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.186	4.26 ng	205500	Naphthalene-d8	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	42
2			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	38
3			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	38
4			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	38
5			Naphthalene, decahydro-2,2-dimet...	166	C12H22	031124-85-3	38



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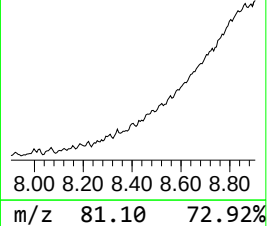
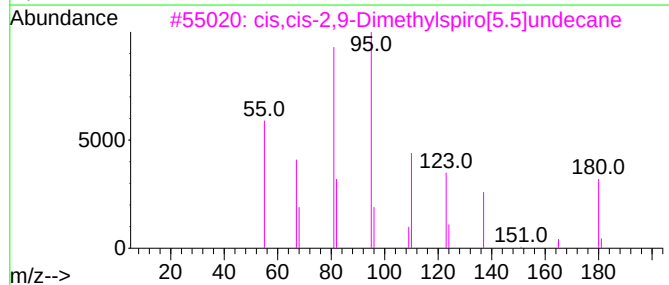
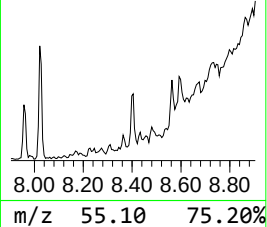
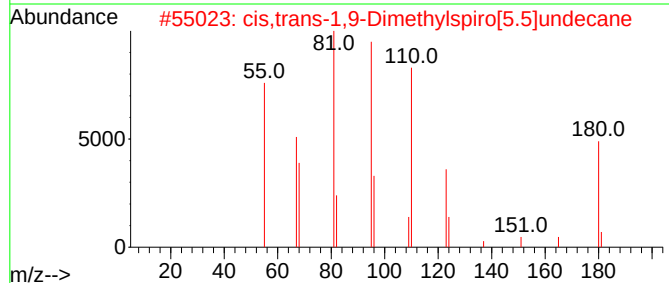
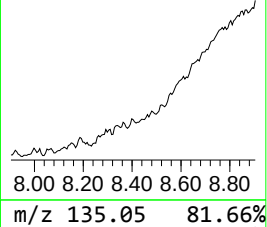
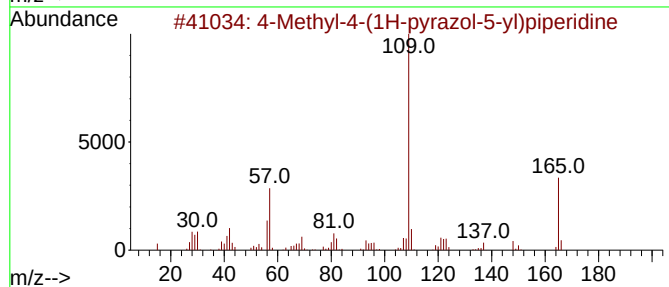
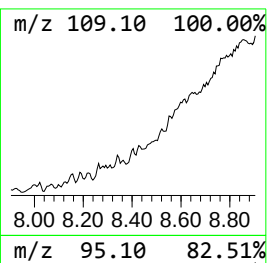
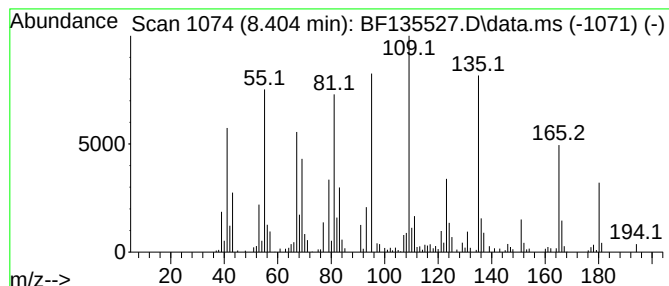
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Peak Number 2 unknown8.404 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.404	4.17 ng	201330	Naphthalene-d8	8.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-4-(1H-pyrazol-5-yl)pipe...	165	C9H15N3	1000460-41-6	38
2			cis,trans-1,9-Dimethylspiro[5.5]...	180	C13H24	1000111-73-3	30
3			cis,cis-2,9-Dimethylspiro[5.5]un...	180	C13H24	095472-51-8	25
4			1-(Hydroxyamino)adamantane	167	C10H17NO	031463-23-7	25
5			2(1H)-Naphthalenone, octahydro-4...	180	C12H20O	051557-64-3	20



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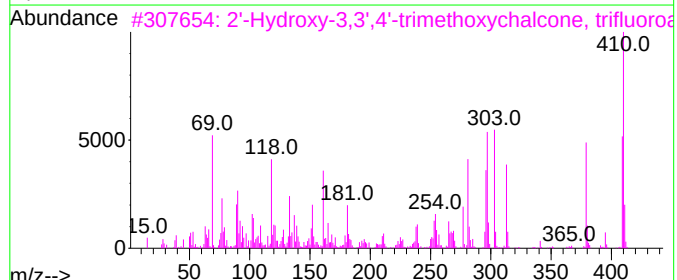
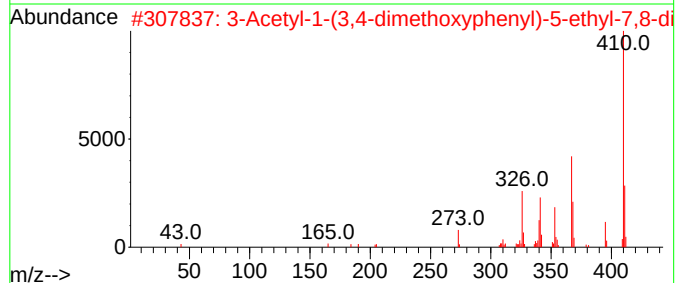
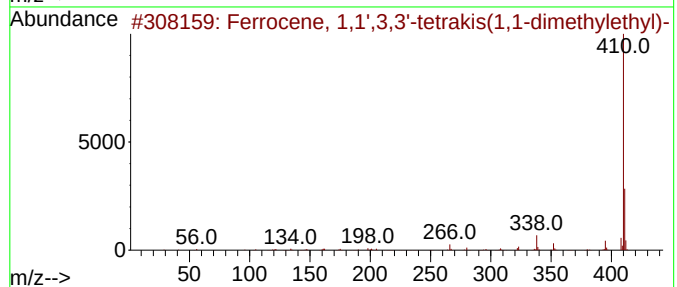
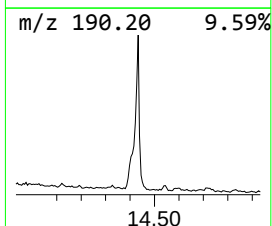
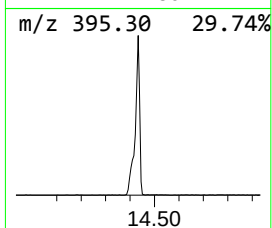
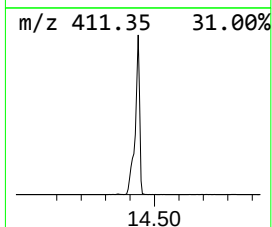
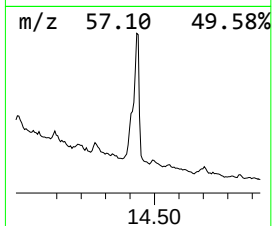
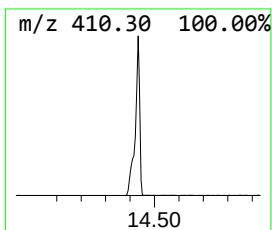
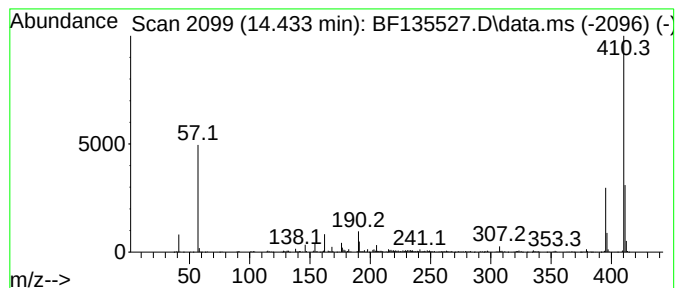
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Peak Number 3 Ferrocene, 1,1',3,3'-tetrak... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.433	20.00 ng	2288450	Chrysene-d12	13.963	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	64
2	3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	64
3	2'-Hydroxy-3,3',4'-trimethoxycha...	410	C20H17F3O6	1010453-84-8	52
4	Di(trimethylene-1-naphthyl)siloxane	410	C26H26OSi2	093241-94-2	43
5	Stigmasta-4,6,22-trien-3.beta.-ol	410	C29H46O	096737-58-5	42



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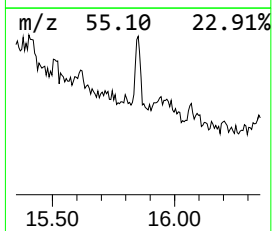
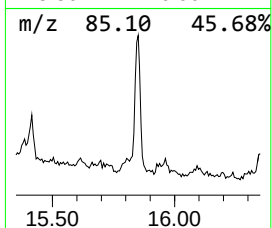
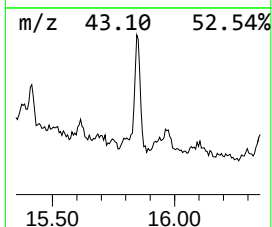
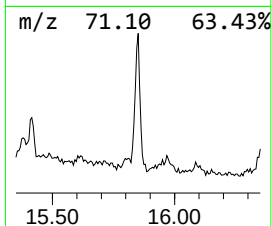
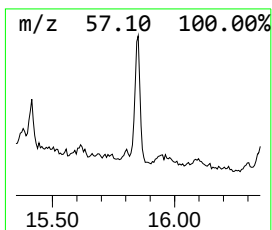
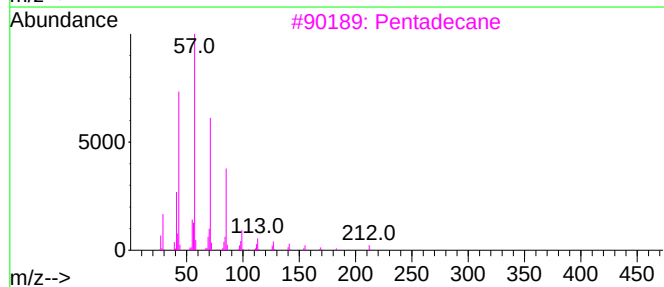
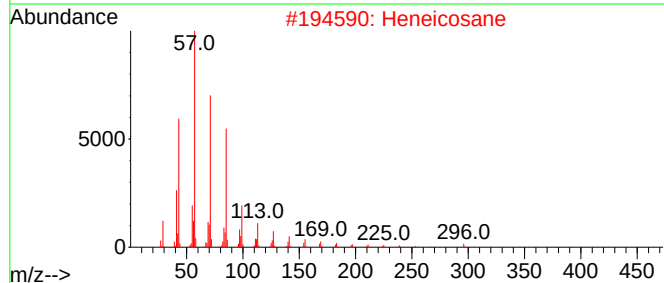
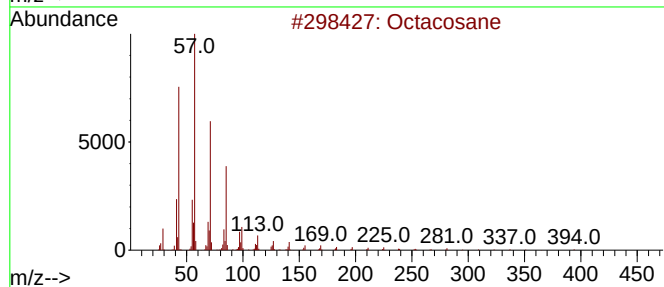
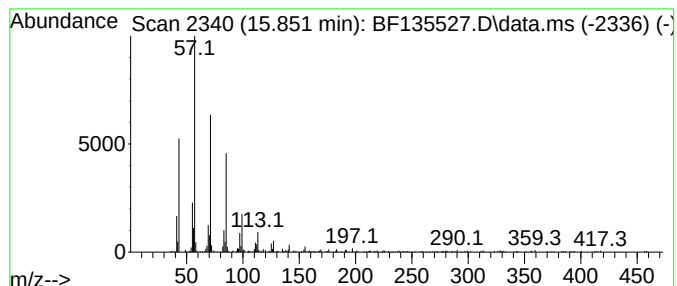
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Peak Number 4 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.851	6.14 ng	308369	Perylene-d12	15.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Pentadecane	212	C15H32	000629-62-9	86
4			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	86
5			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	86



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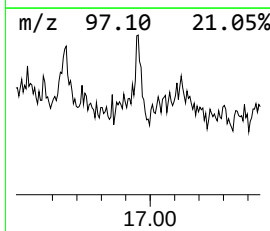
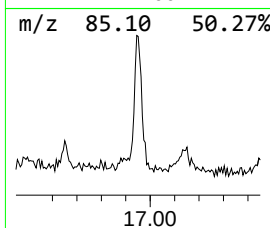
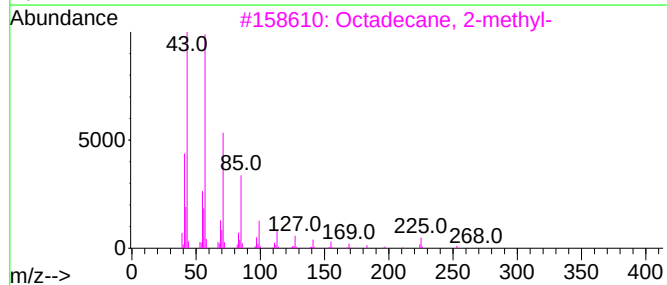
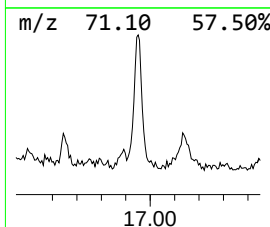
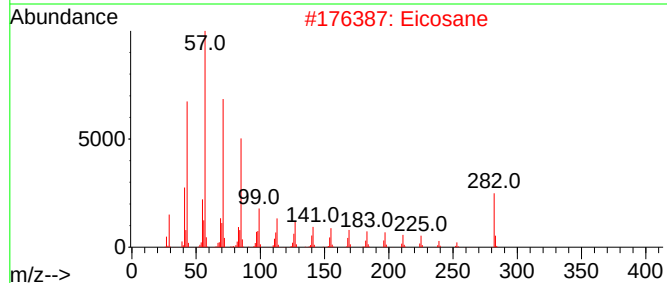
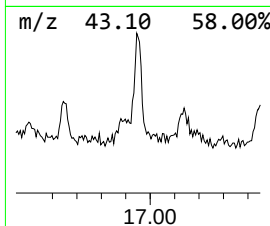
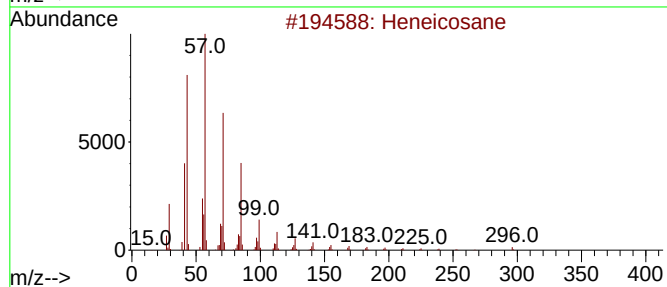
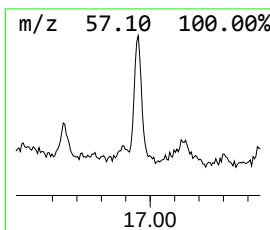
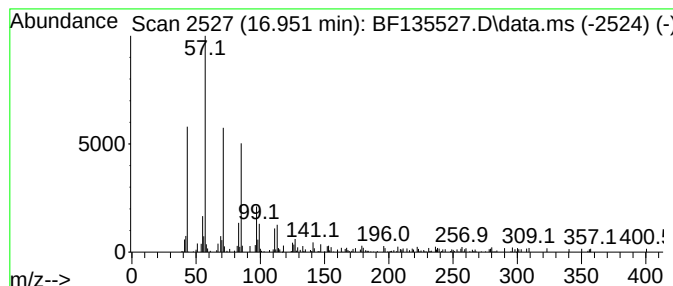
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Peak Number 5 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.951	3.60 ng	180715	Perylene-d12	15.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	81
2			Eicosane	282	C20H42	000112-95-8	76
3			Octadecane, 2-methyl-	268	C19H40	001560-88-9	72
4			Nonadecane	268	C19H40	000629-92-5	72
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	64



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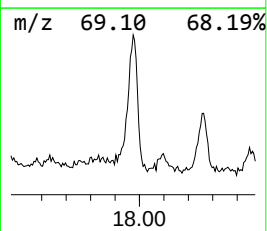
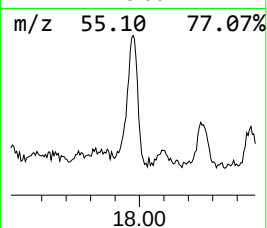
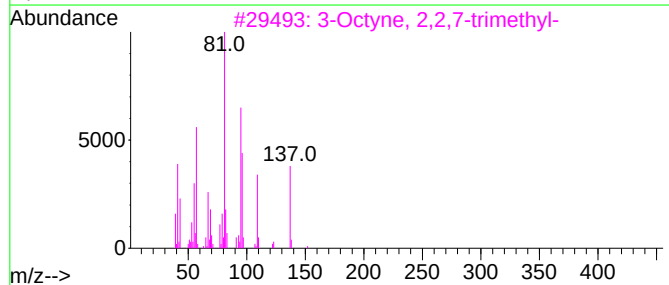
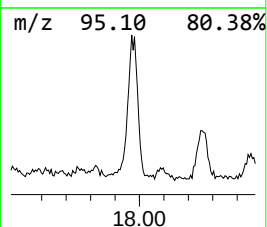
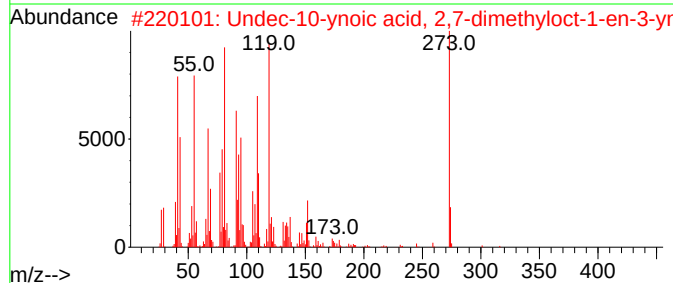
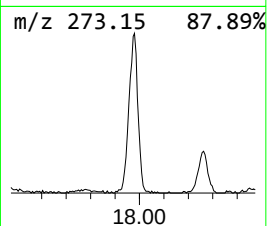
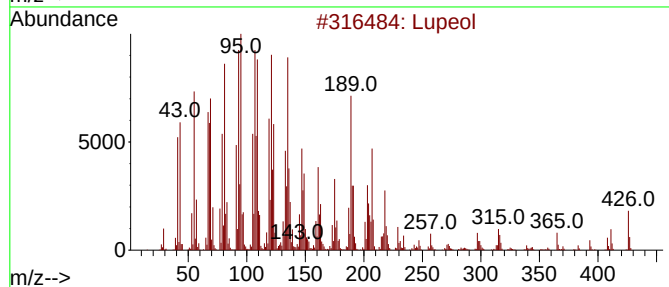
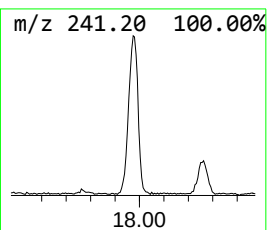
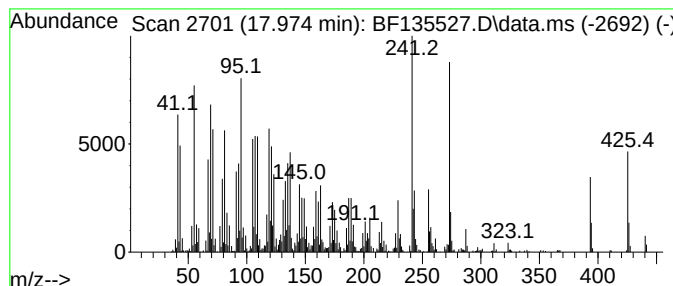
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Peak Number 6 unknown17.974 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	39.05 ng	1959850	Perylene-d12	15.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	47
2			Undec-10-ynoic acid, 2,7-dimethy...	316	C21H32O2	1000406-96-7	27
3			3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	25
4			1-(4-Methyl-6-chloro-quinolin-2-...	273	C14H12ClN3O	111784-26-0	22
5			Crinan-1-ol, (1.alpha.)-	273	C16H19NO3	041928-89-6	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135527.D
Acq On : 02 Oct 2023 15:02
Operator : CG\JU
Sample : 04668-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR251697

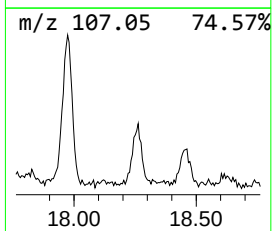
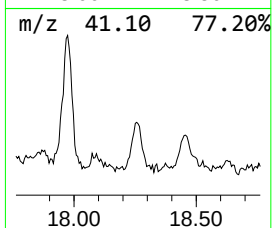
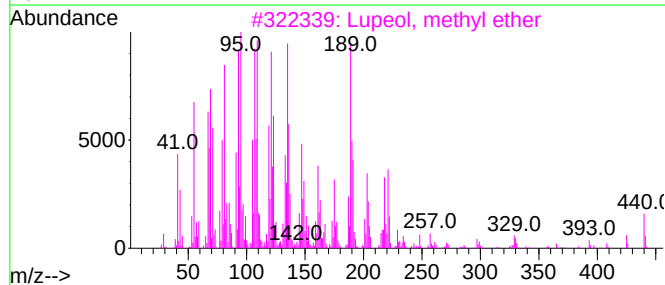
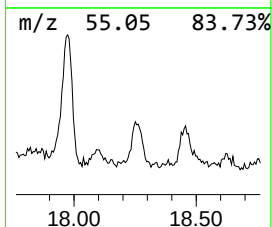
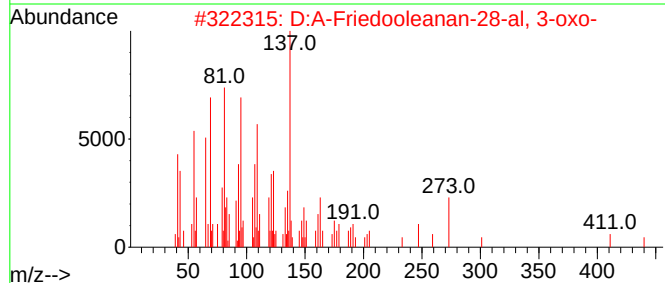
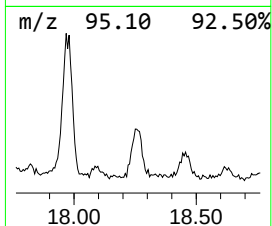
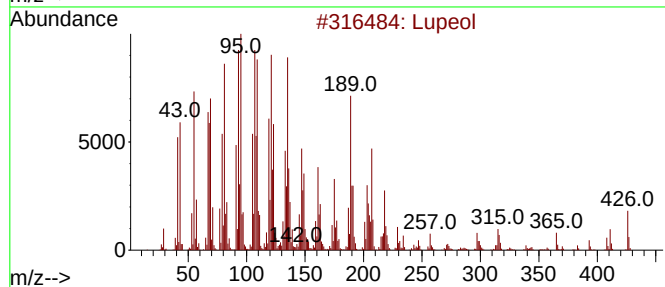
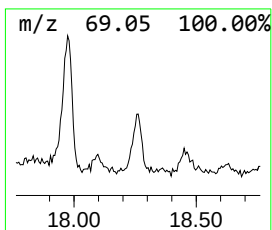
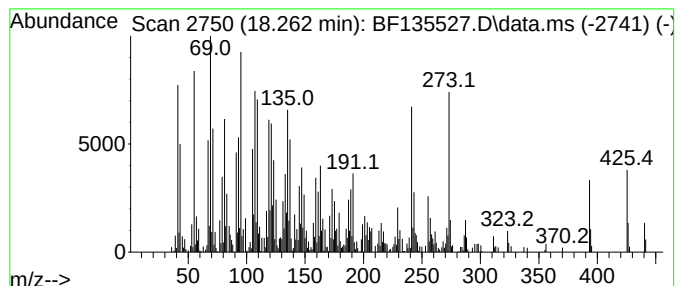
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Lupeol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.262	13.99 ng	702261	Perylene-d12	15.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	50
2			D:A-Friedooleanan-28-al, 3-oxo-	440	C30H48O2	014440-40-5	46
3			Lupeol, methyl ether	440	C31H52O	025279-38-3	42
4			11-Oxo-.beta.-amyrin	440	C30H48O2	038242-02-3	41
5			9,19-Cyclolanost-24-en-3-ol, (3....	426	C30H50O	000469-38-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135527.D
Acq On : 02 Oct 2023 15:02
Operator : CG\JU
Sample : 04668-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

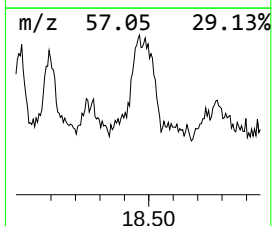
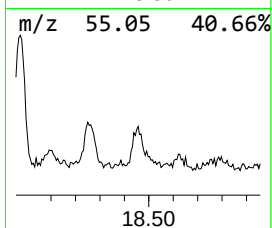
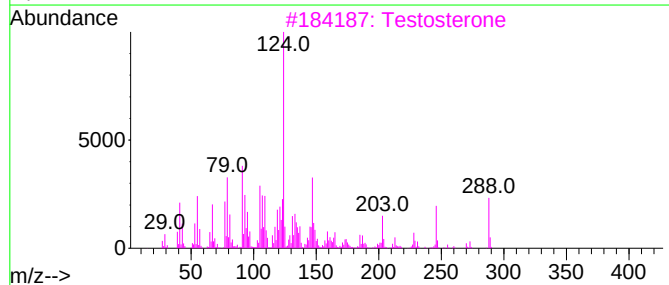
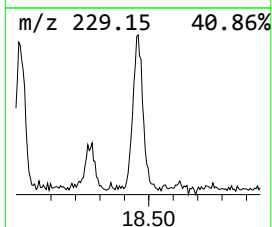
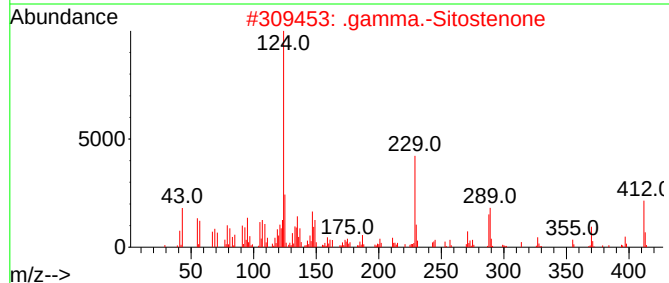
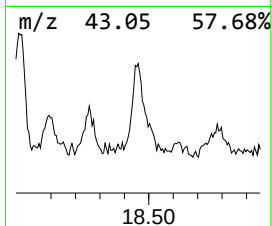
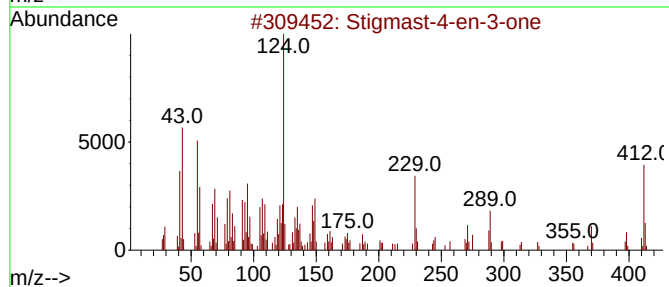
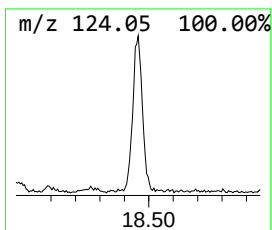
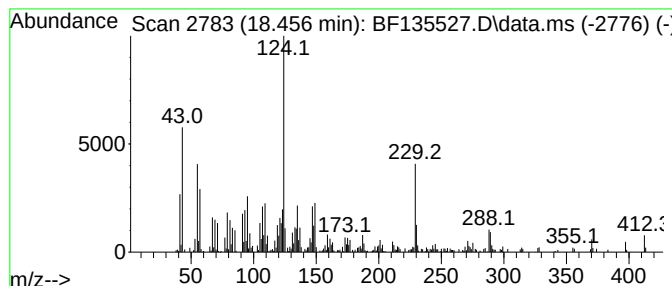
Instrument :
BNA_F
ClientSampleId :
RBR251697

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Stigmast-4-en-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.456	11.99 ng	601822	Perylene-d12		15.403	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Stigmast-4-en-3-one		412	C29H48O	001058-61-3	94
2	.gamma.-Sitostenone		412	C29H48O	084924-96-9	81
3	Testosterone		288	C19H28O2	000058-22-0	80
4	Androst-4-en-3-one, 17-hydroxy-,...		288	C19H28O2	000604-39-7	70
5	7.alpha.-Hydroxytestosterone		304	C19H28O3	000062-83-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100223\
Data File : BF135527.D
Acq On : 02 Oct 2023 15:02
Operator : CG\JU
Sample : 04668-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR251697

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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
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unknown8.404	8.404	4.2	ng	201330	2	8.022	964635	20.0
Ferrocene, 1,1'...	14.433	20.0	ng	2288450	5	13.963	2288450	20.0
Octacosane	15.851	6.1	ng	308369	6	15.403	1003650	20.0
Heneicosane	16.951	3.6	ng	180715	6	15.403	1003650	20.0
unknown17.974	17.974	39.0	ng	1959850	6	15.403	1003650	20.0
Lupeol	18.262	14.0	ng	702261	6	15.403	1003650	20.0
Stigmast-4-en-3...	18.456	12.0	ng	601822	6	15.403	1003650	20.0