

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071620\
 Data File : BF120907.D
 Acq On : 17 Jul 2020 1:49
 Operator : JU/CG
 Sample : L3308-15
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 15

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.840	294	298	304	rVB	37582	49819	1.46%	0.179%
2	5.422	562	567	570	rBV	2890977	2694258	78.92%	9.681%
3	6.440	735	740	743	rBV	2796552	2744309	80.38%	9.861%
4	6.640	771	774	780	rBV	123623	95068	2.78%	0.342%
5	6.816	800	804	807	rBV	1162275	973209	28.51%	3.497%
6	7.375	894	899	902	rBV	2077810	1787898	52.37%	6.424%
7	8.098	1018	1022	1025	rBV	1599839	1291185	37.82%	4.640%
8	9.175	1201	1205	1208	rBV	3866566	3269748	95.77%	11.749%
9	9.510	1259	1262	1265	rBV	60222	45904	1.34%	0.165%
10	9.563	1268	1271	1275	rBV	773726	658972	19.30%	2.368%
11	9.851	1316	1320	1323	rBV	1921485	1488290	43.59%	5.348%
12	10.633	1449	1453	1457	rBV	2188007	2134063	62.51%	7.668%
13	11.333	1568	1572	1575	rBV	1900438	1528008	44.76%	5.490%
14	11.863	1659	1662	1667	rBV	80446	84175	2.47%	0.302%
15	12.033	1685	1691	1697	rBV6	26244	41000	1.20%	0.147%
16	12.586	1782	1785	1792	rBV2	44115	42189	1.24%	0.152%
17	12.921	1837	1842	1845	rBV	3685100	3414032	100.00%	12.267%
18	12.980	1845	1852	1863	rVB	63662	252958	7.41%	0.909%
19	13.351	1912	1915	1917	rBV	121541	95047	2.78%	0.342%
20	13.616	1957	1960	1965	rVB6	37003	38488	1.13%	0.138%
21	13.816	1991	1994	2001	rBV	568927	601057	17.61%	2.160%
22	13.968	2016	2020	2023	rBV	1301171	1185262	34.72%	4.259%
23	14.145	2047	2050	2054	rVB4	31071	40227	1.18%	0.145%
24	14.451	2099	2102	2109	rVB	188890	207025	6.06%	0.744%
25	14.892	2175	2177	2182	rVB3	37052	41209	1.21%	0.148%
26	15.086	2206	2210	2212	rBV	132896	158171	4.63%	0.568%
27	15.415	2261	2266	2271	rBV	889932	1042099	30.52%	3.744%
28	15.657	2303	2307	2310	rBV	54265	78533	2.30%	0.282%
29	15.886	2342	2346	2350	rBV	79529	103512	3.03%	0.372%
30	15.933	2350	2354	2362	rBV2	142914	274264	8.03%	0.985%
31	16.662	2475	2478	2485	rVB4	42619	67228	1.97%	0.242%
32	17.421	2601	2607	2617	rBV2	215696	502643	14.72%	1.806%
33	17.751	2658	2663	2669	rBV6	72280	146874	4.30%	0.528%
34	17.874	2681	2684	2693	rVB2	62992	122088	3.58%	0.439%

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15

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-BF071620.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.998	2700	2705	2714	rVB5	119627	304006	8.90%	1.092%
36	18.427	2774	2778	2793	rVB5	88615	227385	6.66%	0.817%

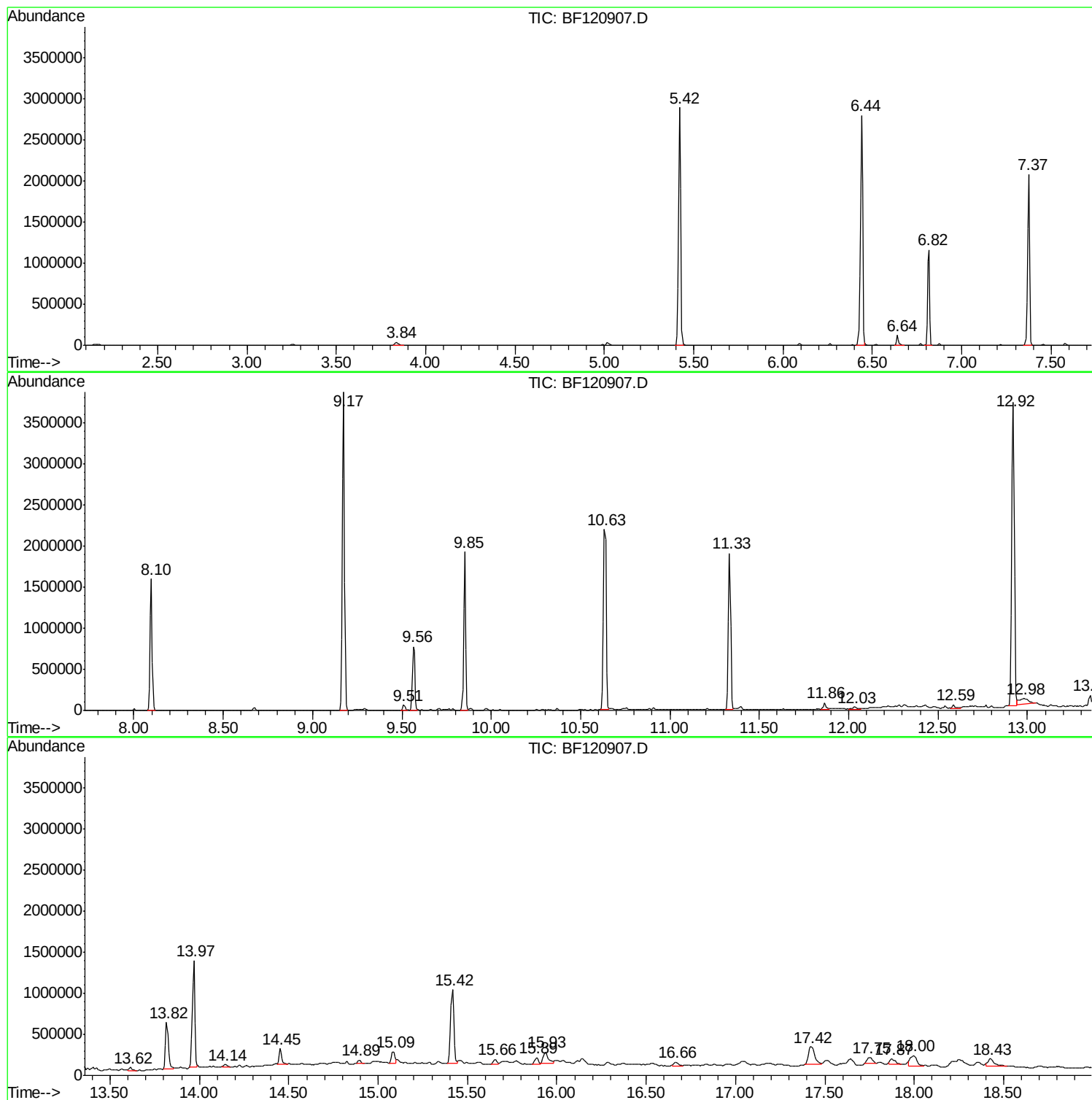
Sum of corrected areas: 27830203

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15

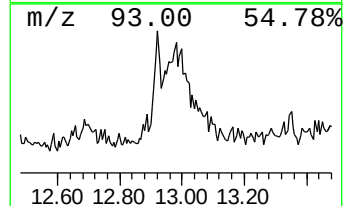
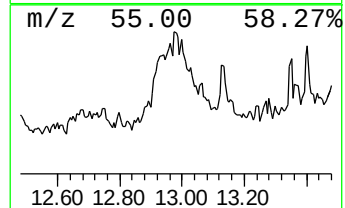
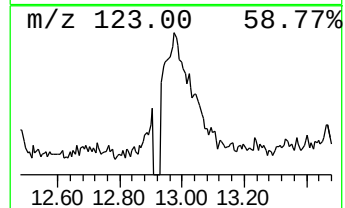
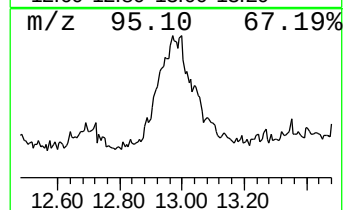
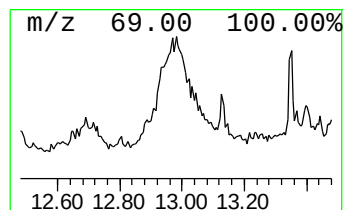
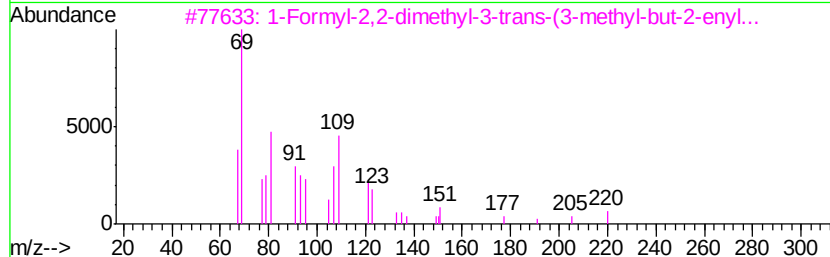
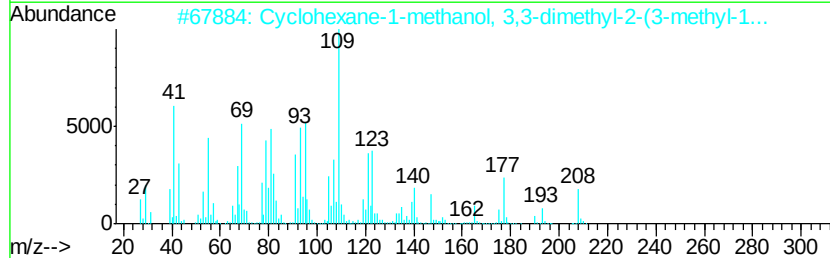
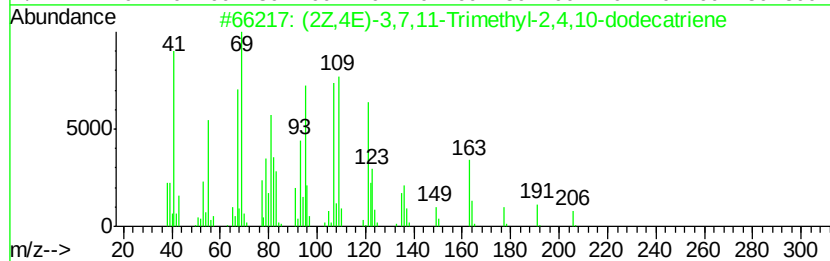
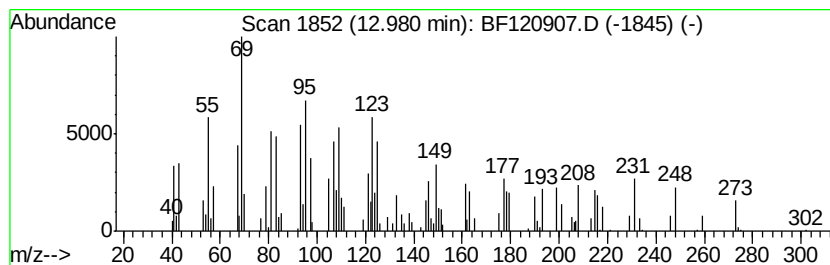
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown12.98 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	4.27 ng	252958	Chrysene-d12	13.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	38		
2	Cyclohexane-1-methanol, 3,3-dime...	208	C14H24O	1000196-01-5	38		
3	1-Formyl-2,2-dimethyl-3-trans-(3...	220	C15H24O	1000144-09-7	35		
4	3,7-Decadiyne, 2,2,5,5,6,6,9,9-o...	246	C18H30	017553-35-4	25		
5	3-Heptene, 2,2,3,5,6-pentamethyl-	168	C12H24	116164-06-8	22		



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

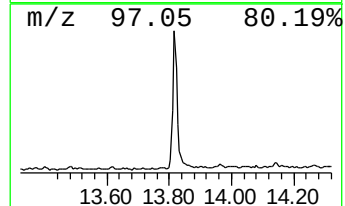
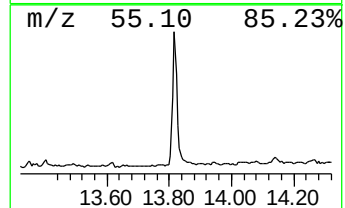
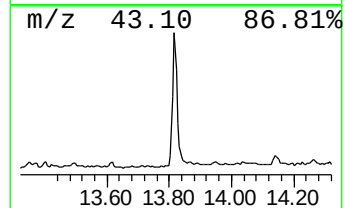
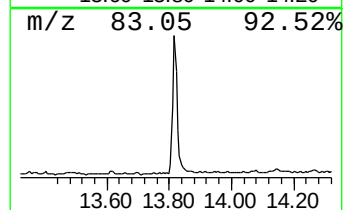
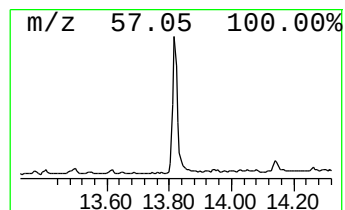
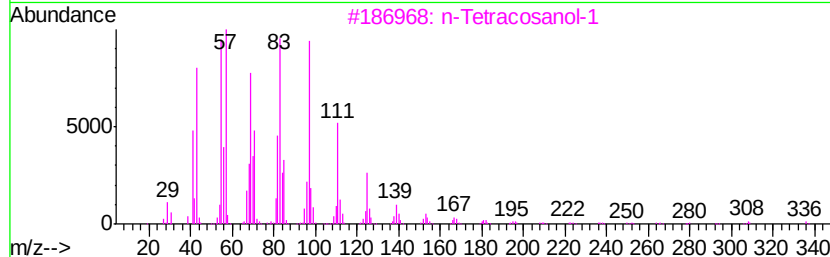
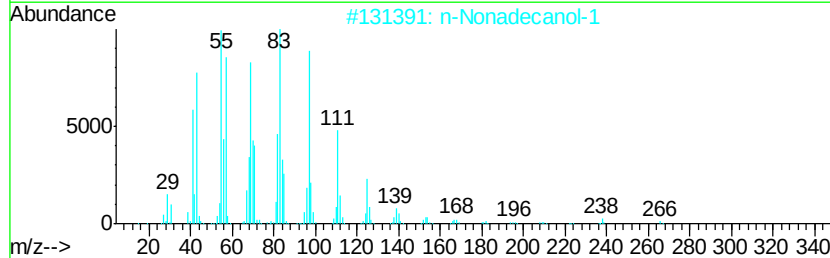
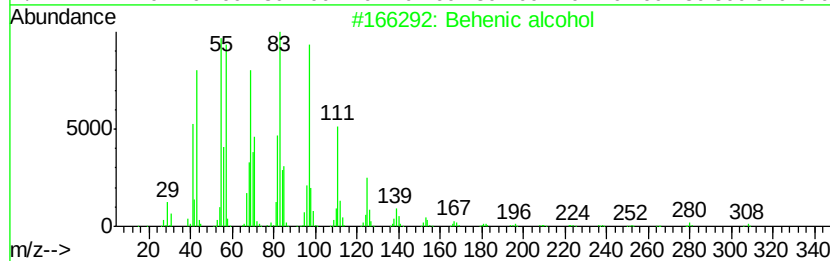
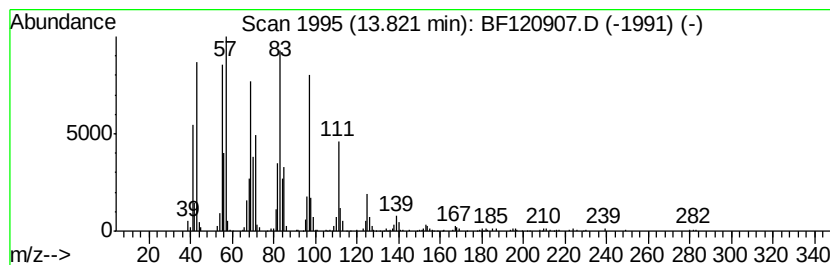
Instrument :
BNA_F
ClientSampleId :
15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.82	10.14 ng	601057	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

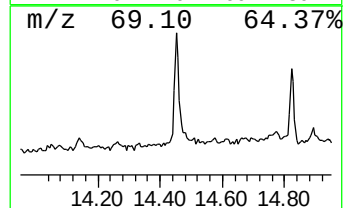
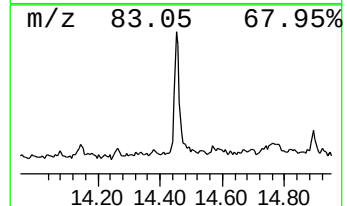
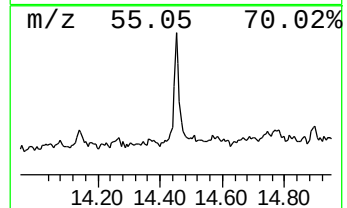
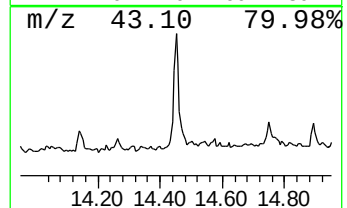
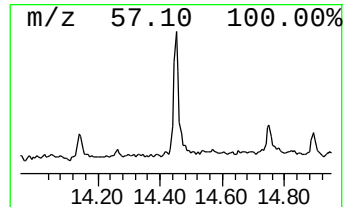
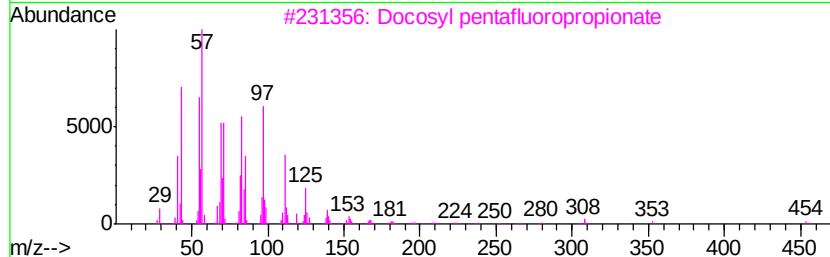
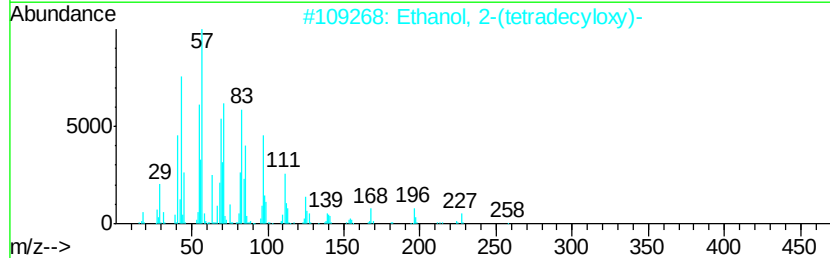
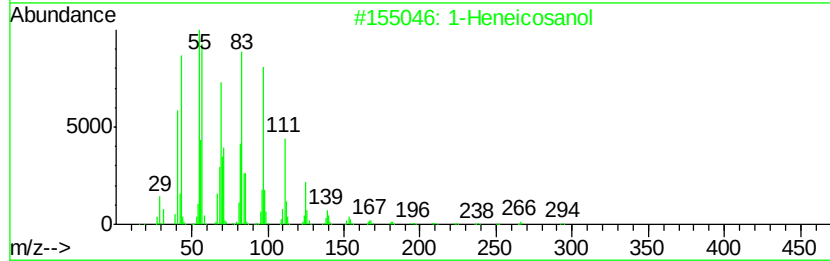
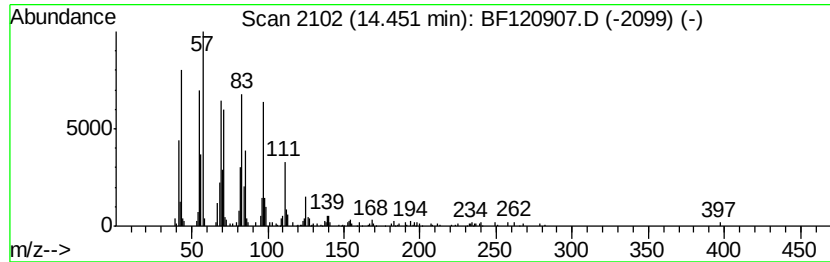
Instrument :
BNA_F
ClientSampleId :
15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.49 ng	207025	Chrysene-d12	13.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 93
2		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 91
3		Docosyl pentafluoropropionate	472 C25H45F5O2	1000351-80-9 91
4		Heptafluorobutyric acid, n-octadecyl-	466 C22H37F7O2	000400-57-7 91
5		Eicosyl pentafluoropropionate	444 C23H41F5O2	1000351-80-8 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15

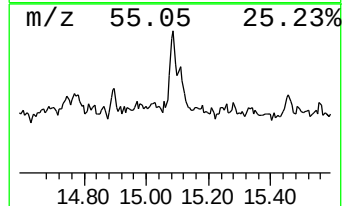
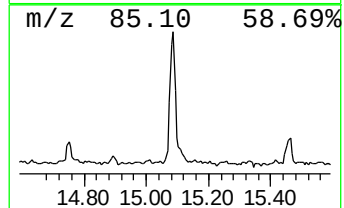
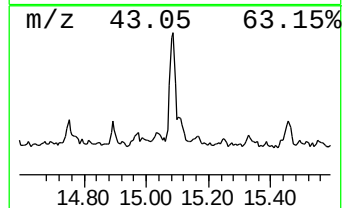
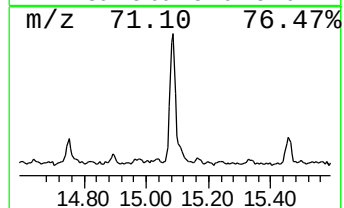
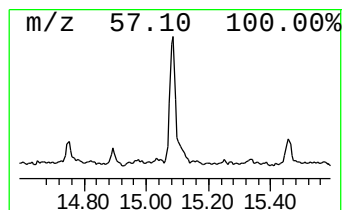
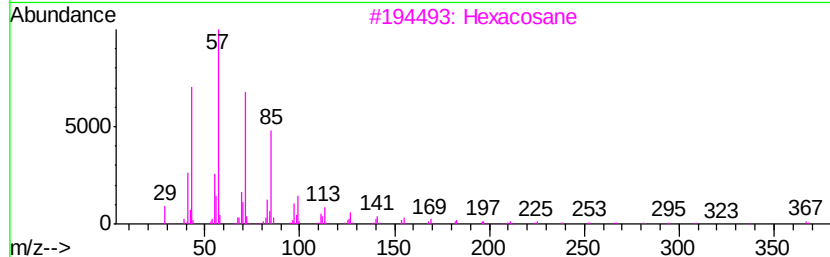
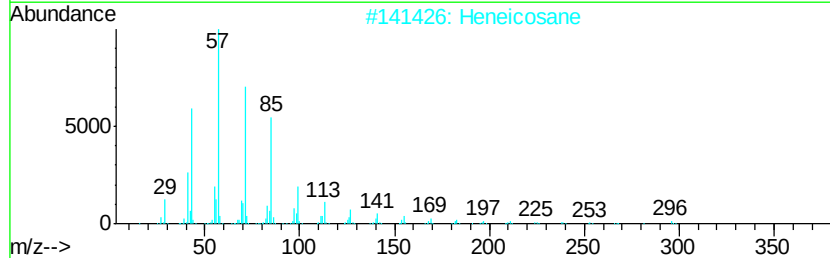
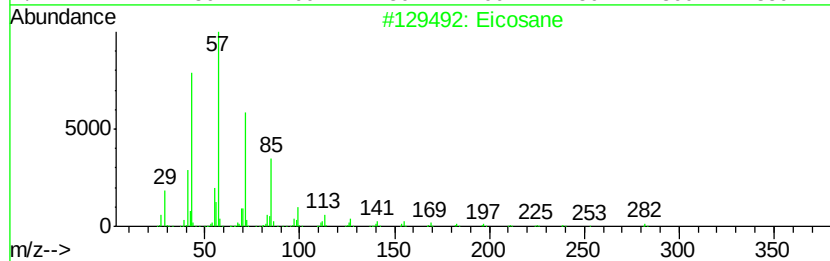
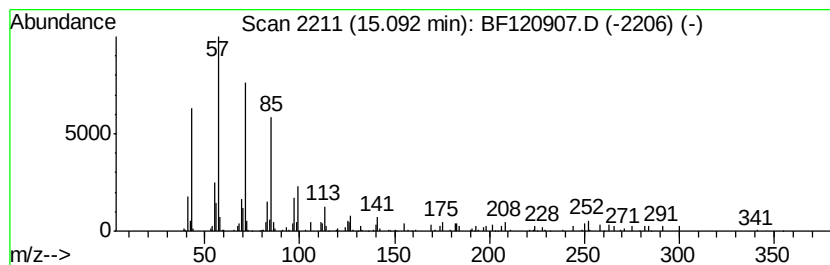
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.04 ng	158171	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

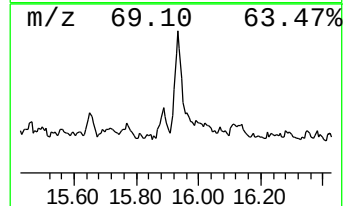
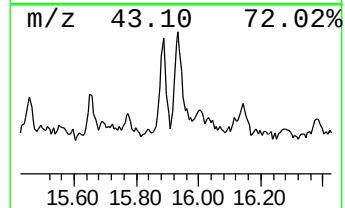
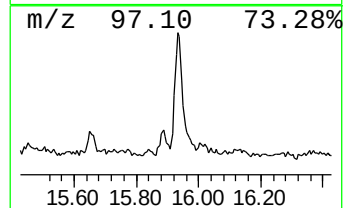
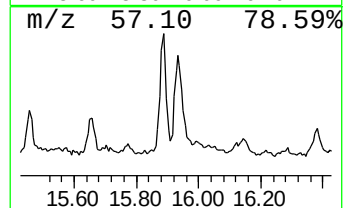
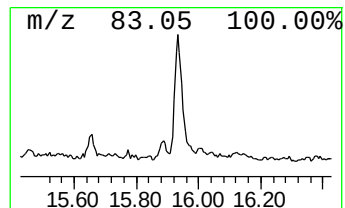
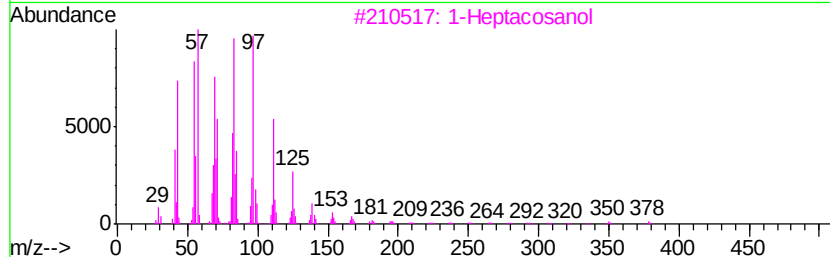
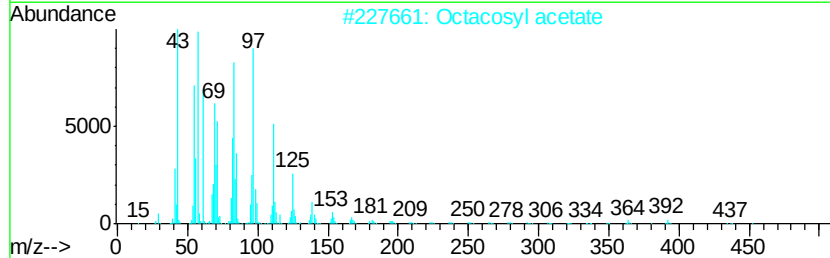
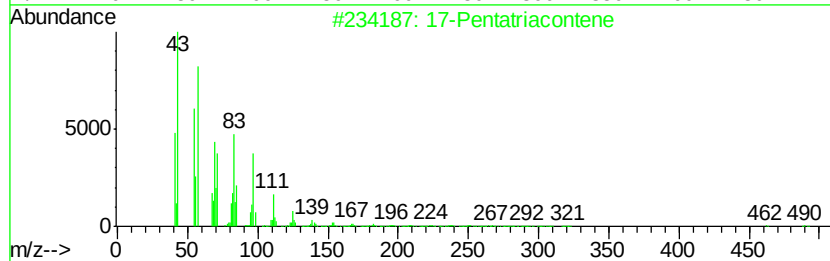
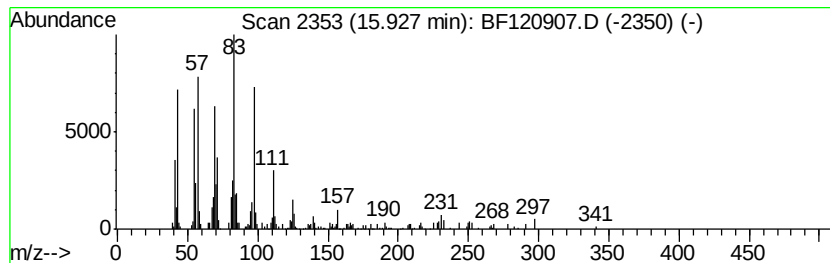
Instrument :
BNA_F
ClientSampleId :
15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.93	5.26 ng	274264	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	76
2	Octacosyl acetate	452	C30H60O2	018206-97-8	70
3	1-Heptacosanol	396	C27H56O	002004-39-9	70
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	70
5	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

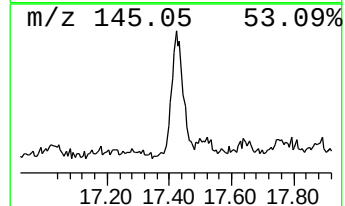
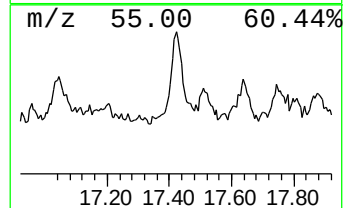
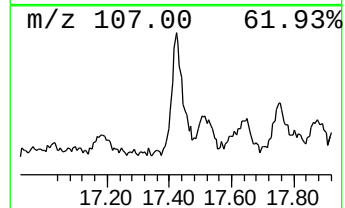
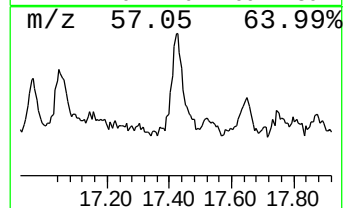
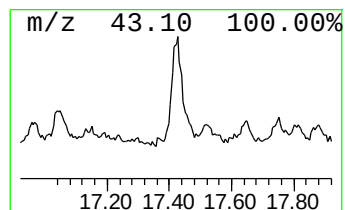
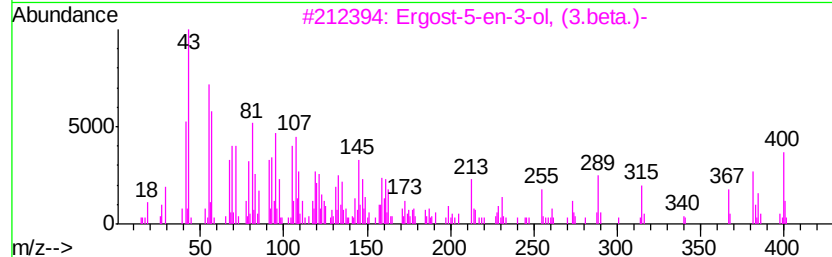
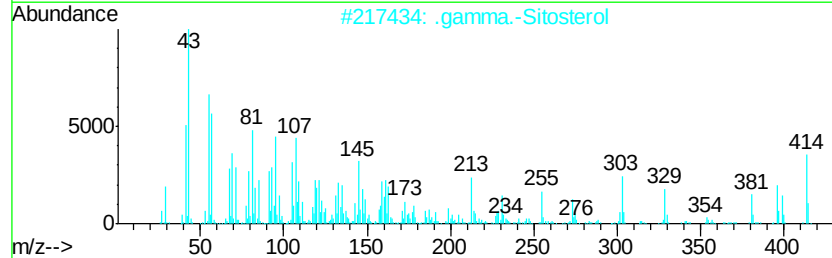
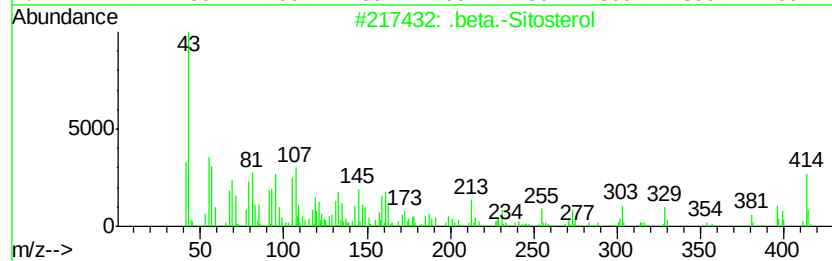
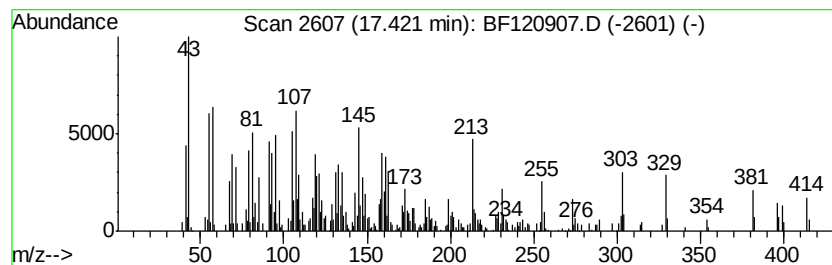
Instrument :
BNA_F
ClientSampleId :
15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 .beta.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.42	9.65 ng	502643	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
3	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	43
4	Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	38
5	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

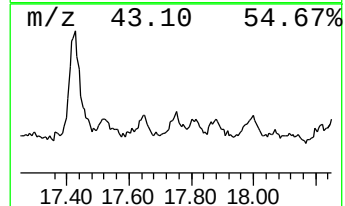
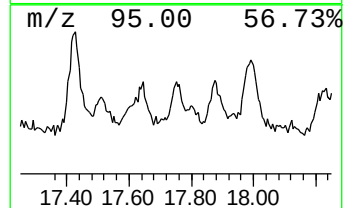
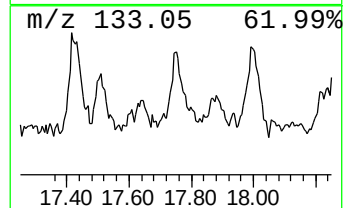
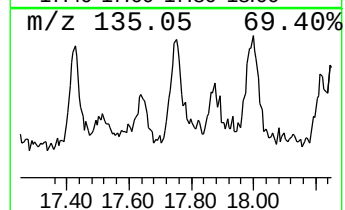
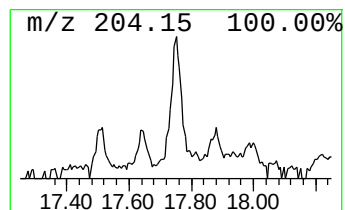
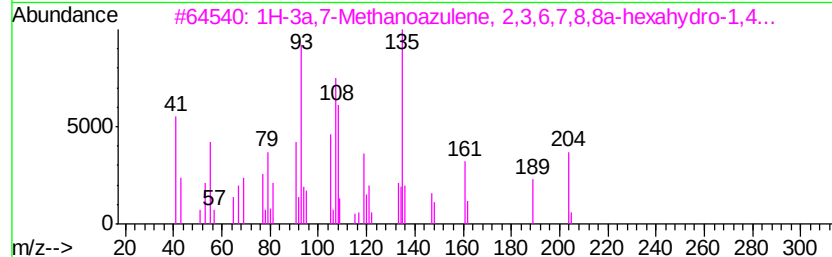
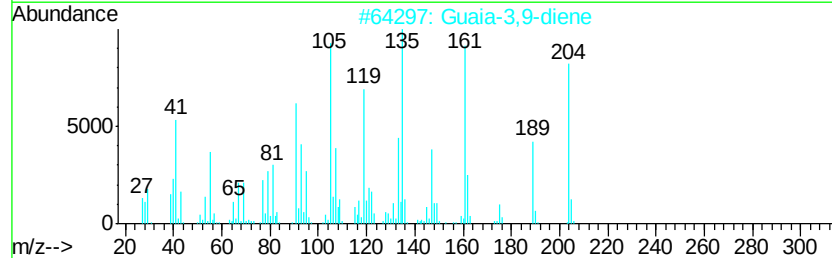
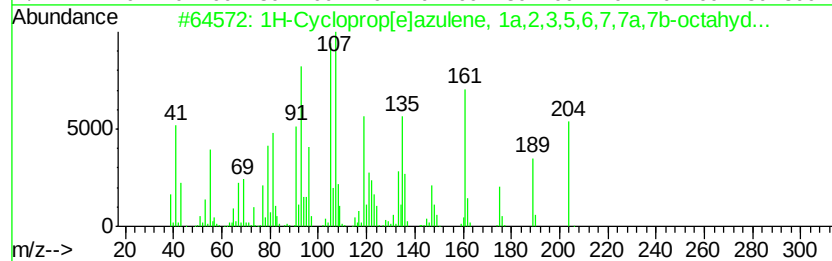
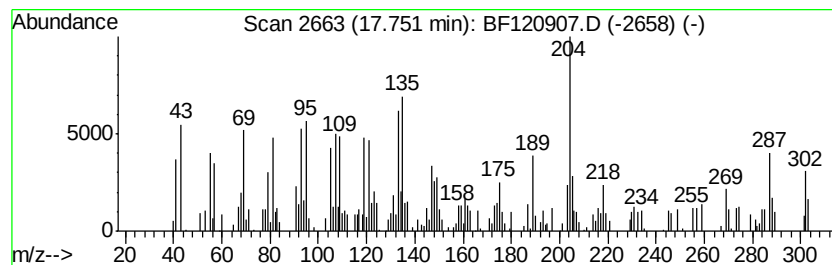
Instrument :
BNA_F
ClientSampled :
15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	2.82 ng	146874	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1H-Cycloprop[elazulene, 1a,2,3,5...	204 C15H24	021747-46-6 64
2		Guaia-3,9-diene	204 C15H24	000489-83-8 49
3		1H-3a,7-Methanoazulene, 2,3,6,7,...	204 C15H24	000560-32-7 43
4		Aciphyllene	204 C15H24	087745-31-1 41
5		2,2,6-Trimethyl-1-(2-methyl-cycl...	218 C15H22O	1000188-72-8 25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15

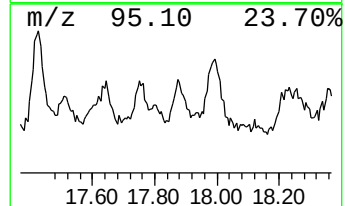
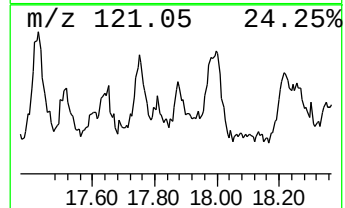
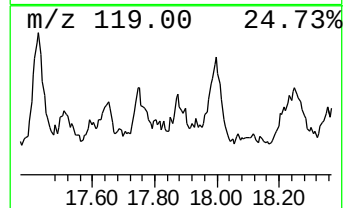
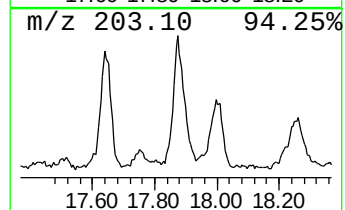
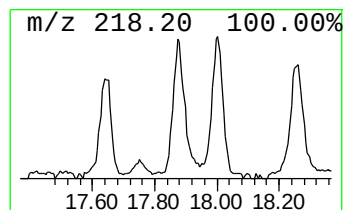
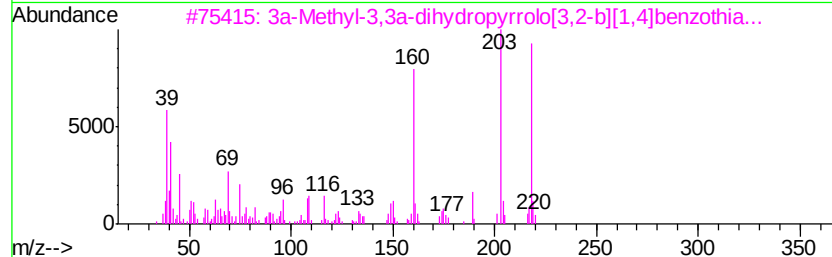
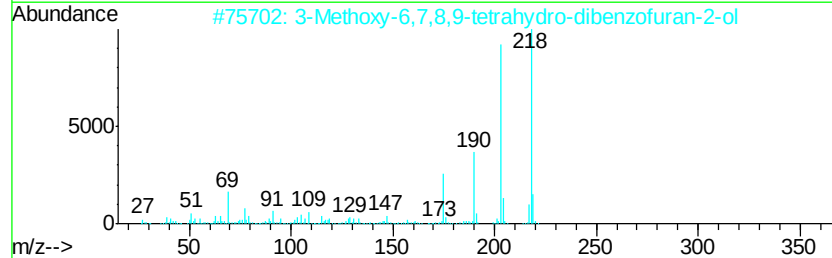
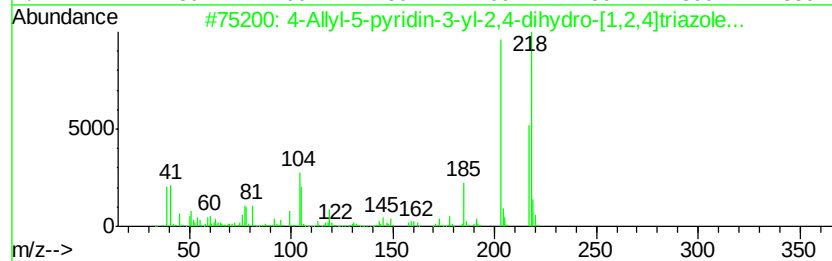
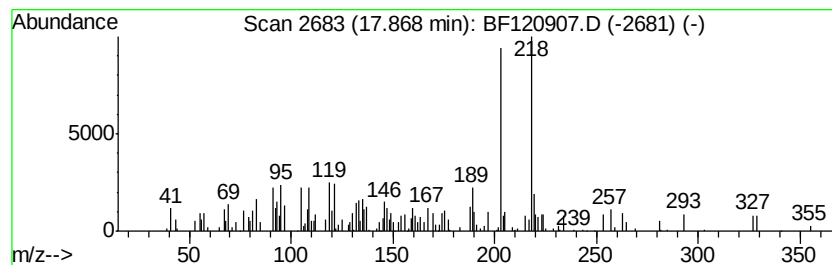
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4-Allyl-5-pyridin-3-yl-2,4-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.87	2.34 ng	122088	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Allyl-5-pyridin-3-yl-2,4-dihyd...	218	C10H10N4S	1000300-40-5	60
2		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	53
3		3a-Methyl-3,3a-dihydropyrrolo[3,...	218	C11H10N2OS	017163-68-7	52
4		3H-1,2,4-Triazole-3-thione, 2,4-...	218	C10H10N4S	091813-63-7	49
5		8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

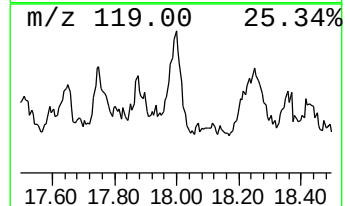
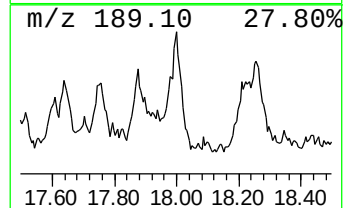
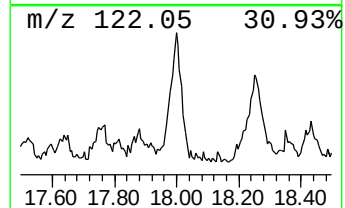
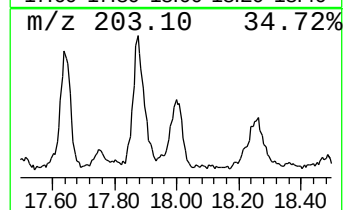
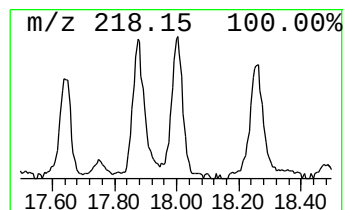
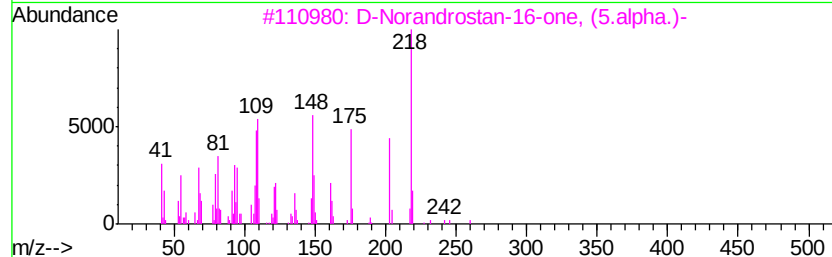
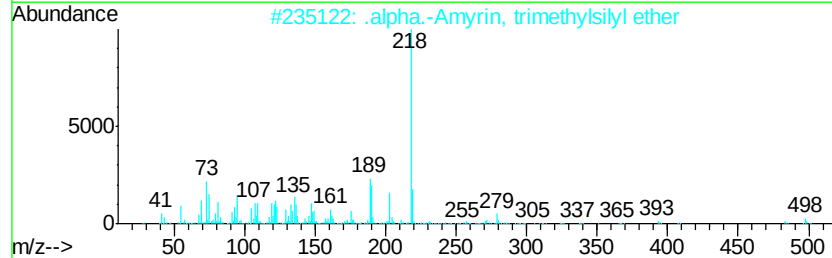
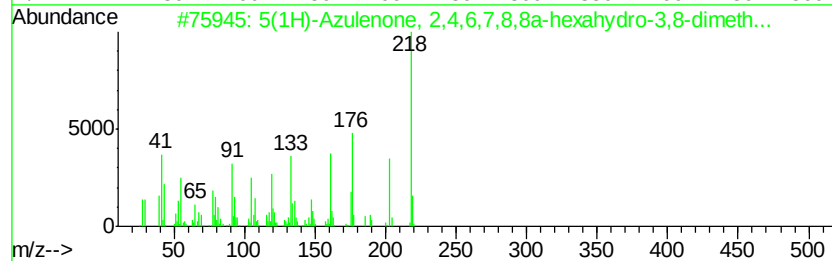
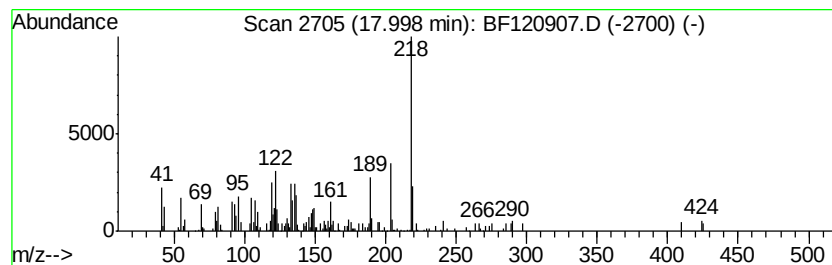
Instrument :
BNA_F
ClientSampleId :
15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 5(1H)-Azulenone, 2,4,6,7,8,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.00	5.83 ng	304006	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218 C15H22O	006754-66-1	64
2	.alpha.-Amyrin, trimethylsilyl e...	498 C33H58OSi	1000374-76-6	53
3	D-Norandrostan-16-one, (5.alpha.)-	260 C18H28O	032319-06-5	47
4	Benzo[b]naphtho[2,3-d]furan	218 C16H10O	000243-42-5	46
5	4,4,6a,6b,8a,11,11,14b-Octamethy...	424 C30H48O	1000194-62-4	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071620\
Data File : BF120907.D
Acq On : 17 Jul 2020 1:49
Operator : JU/CG
Sample : L3308-15
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
15

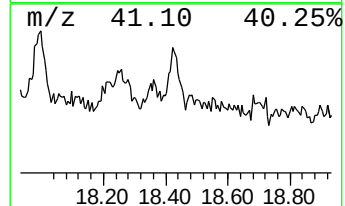
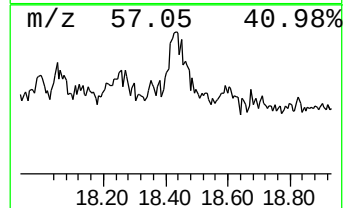
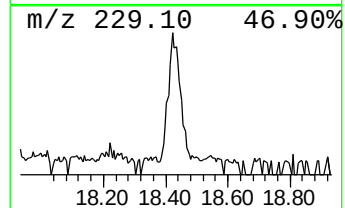
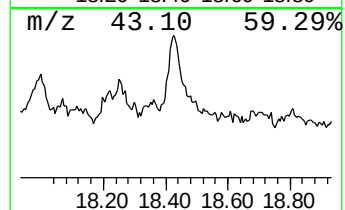
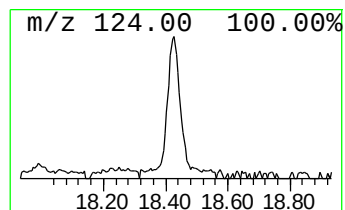
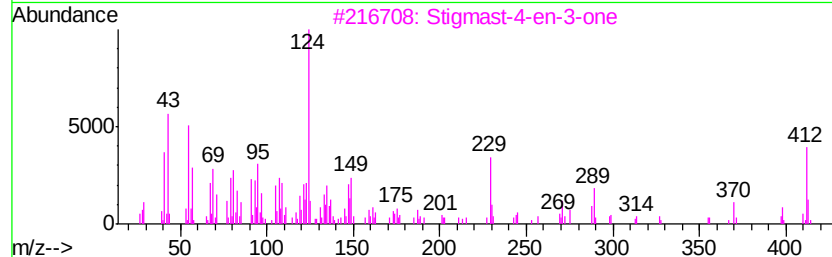
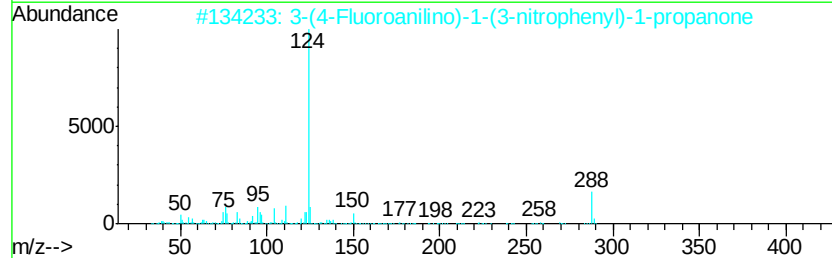
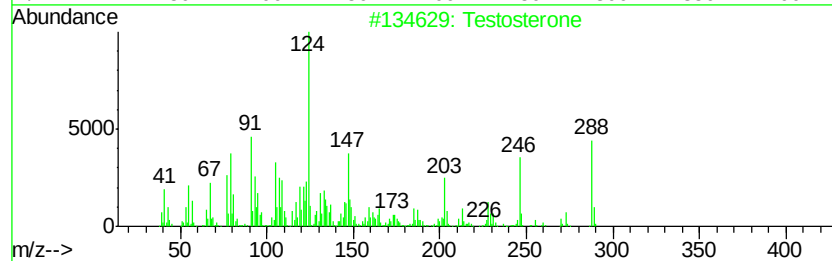
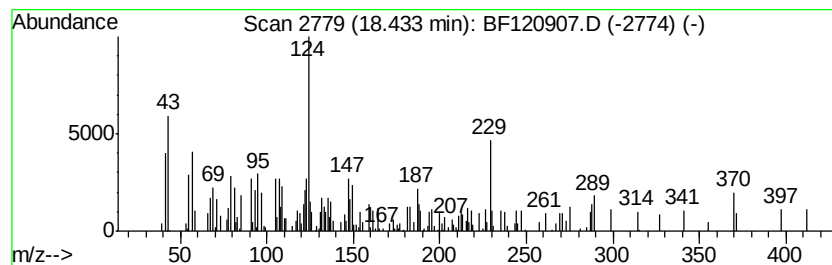
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown18.43 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	4.36 ng	227385	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Testosterone	288	C19H28O2	000058-22-0	46
2		3-(4-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	350039-84-8	46
3		Stigmast-4-en-3-one	412	C29H48O	001058-61-3	46
4		3-(3-Fluoroanilino)-1-(3-nitroph...	288	C15H13FN2O3	300726-64-1	46
5		Homatropine	275	C16H21NO3	000087-00-3	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071620\
 Data File : BF120907.D
 Acq On : 17 Jul 2020 1:49
 Operator : JU/CG
 Sample : L3308-15
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071620.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
unknown12.98	12.98	4.3	ng	252958	5	13.97	1185260	20.0
Behenic alcohol	13.82	10.1	ng	601057	5	13.97	1185260	20.0
1-Heneicosanol	14.45	3.5	ng	207025	5	13.97	1185260	20.0
Eicosane	15.09	3.0	ng	158171	6	15.42	1042100	20.0
17-Pentatriacontene	15.93	5.3	ng	274264	6	15.42	1042100	20.0
.beta.-Sitosterol	17.42	9.7	ng	502643	6	15.42	1042100	20.0
1H-Cycloprop[e]az...	17.75	2.8	ng	146874	6	15.42	1042100	20.0
4-Allyl-5-pyridin...	17.87	2.3	ng	122088	6	15.42	1042100	20.0
5(1H)-Azulenone, ...	18.00	5.8	ng	304006	6	15.42	1042100	20.0
unknown18.43	18.43	4.4	ng	227385	6	15.42	1042100	20.0