

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071720\
 Data File : BF120916.D
 Acq On : 17 Jul 2020 12:02
 Operator : JU/CG
 Sample : L3308-22
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 22

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	5.034	498	501	506	rVB	31692	38437	1.02%	0.122%
2	5.428	563	568	571	rBV	2993911	3015245	79.90%	9.593%
3	6.445	735	741	744	rBV	2748323	3016820	79.94%	9.598%
4	6.640	771	774	780	rBV	43150	43650	1.16%	0.139%
5	6.816	800	804	807	rBV	1406270	1187569	31.47%	3.778%
6	7.375	894	899	902	rBV	2132490	1986399	52.64%	6.320%
7	8.098	1017	1022	1025	rBV	1926724	1566748	41.52%	4.984%
8	9.175	1200	1205	1208	rBV	3911197	3459343	91.67%	11.006%
9	9.563	1267	1271	1275	rBV	659910	624377	16.54%	1.986%
10	9.851	1315	1320	1323	rBV	2180526	1779285	47.15%	5.661%
11	10.639	1449	1454	1457	rBV	2299770	2244743	59.48%	7.141%
12	11.333	1568	1572	1576	rBV	2079719	1841012	48.78%	5.857%
13	11.392	1579	1582	1586	rVB4	35869	39509	1.05%	0.126%
14	11.869	1659	1663	1671	rBV	221325	239905	6.36%	0.763%
15	12.316	1736	1739	1741	rBV	75295	71374	1.89%	0.227%
16	12.586	1783	1785	1792	rVB3	63312	76051	2.02%	0.242%
17	12.921	1837	1842	1845	rBV	3822607	3773888	100.00%	12.006%
18	13.004	1845	1856	1858	rBV2	280551	802673	21.27%	2.554%
19	13.351	1912	1915	1925	rBV4	124032	163166	4.32%	0.519%
20	13.498	1937	1940	1944	rVB2	41112	43222	1.15%	0.138%
21	13.821	1991	1995	2003	rBV	897811	1044932	27.69%	3.324%
22	13.968	2016	2020	2023	rBV	1651423	1417000	37.55%	4.508%
23	14.145	2047	2050	2055	rBV3	53064	65346	1.73%	0.208%
24	14.457	2099	2103	2114	rVB	241847	340560	9.02%	1.083%
25	15.086	2206	2210	2213	rBV	152002	173888	4.61%	0.553%
26	15.415	2261	2266	2270	rBV2	963493	1175451	31.15%	3.740%
27	15.886	2343	2346	2350	rVB	80457	96653	2.56%	0.307%
28	15.939	2350	2355	2363	rBV	289742	532046	14.10%	1.693%
29	17.433	2603	2609	2619	rBV3	185341	441982	11.71%	1.406%
30	18.227	2738	2744	2746	rBV6	59513	131242	3.48%	0.418%

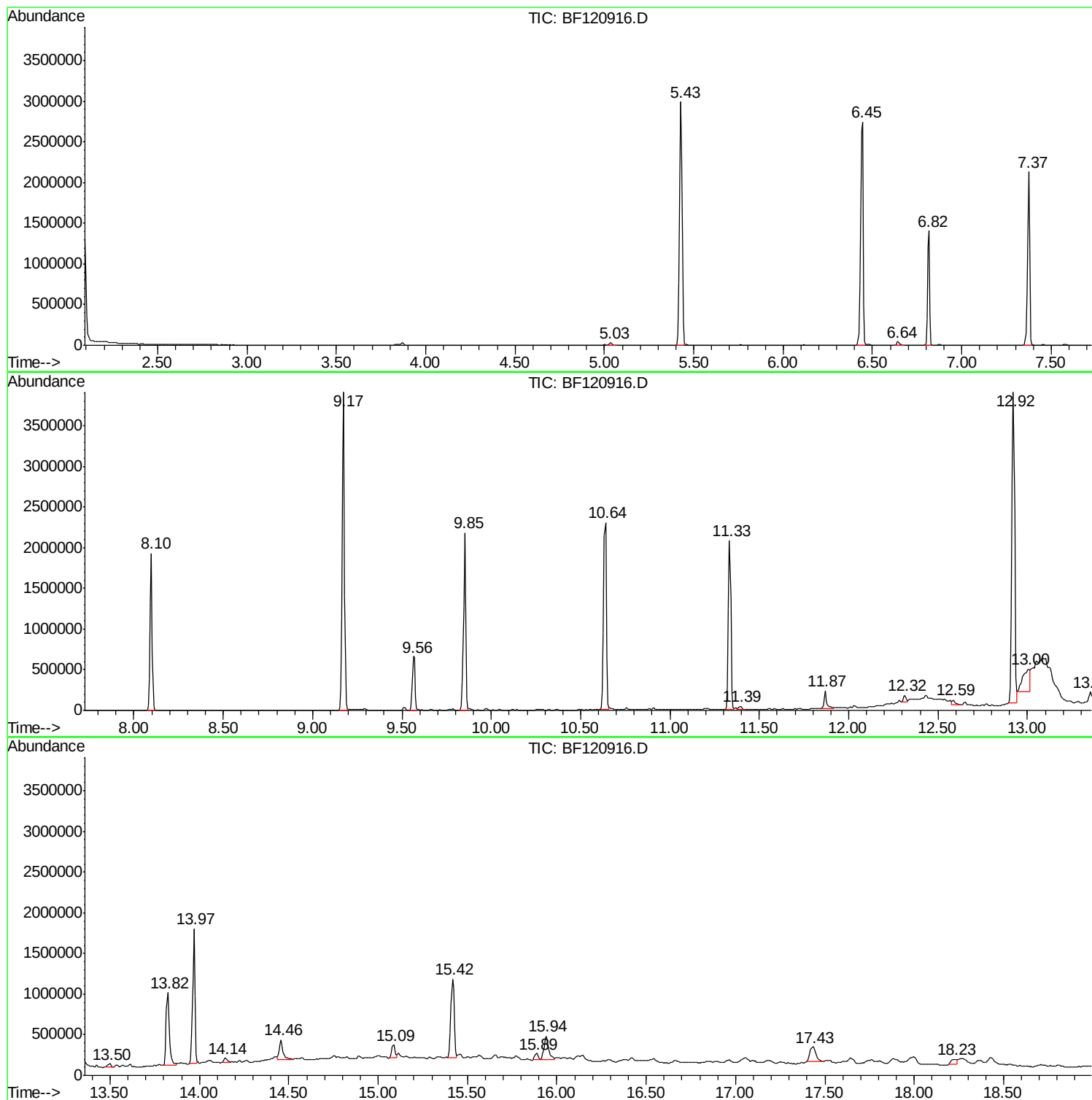
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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
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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



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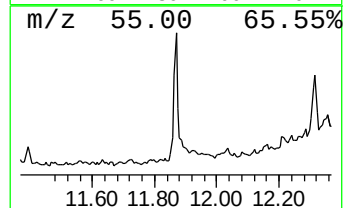
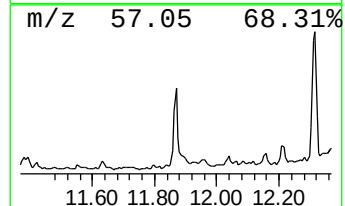
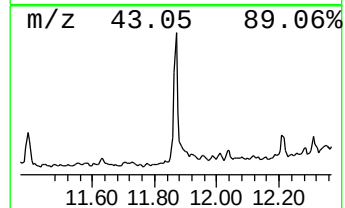
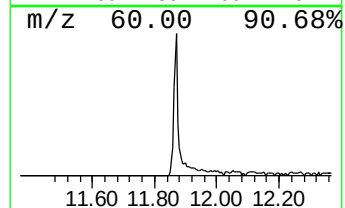
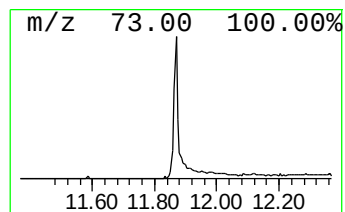
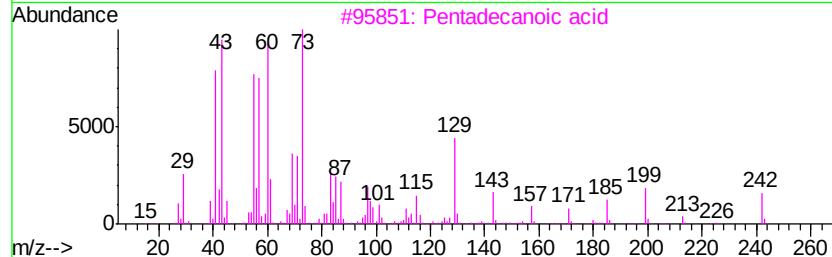
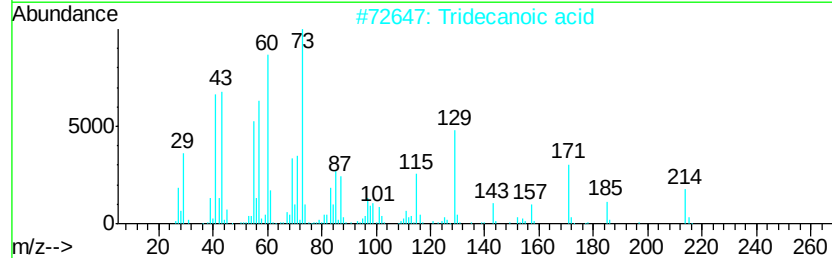
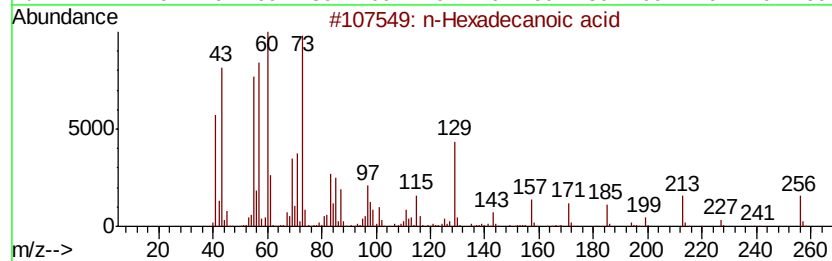
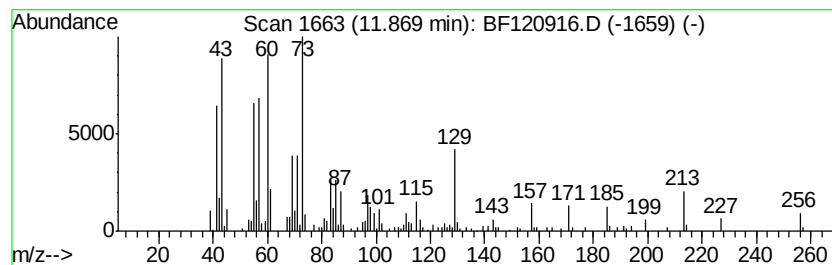
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.87	2.61 ng	239905	Phenanthrene-d10		11.33	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	68



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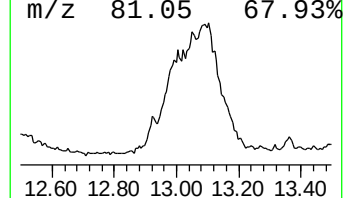
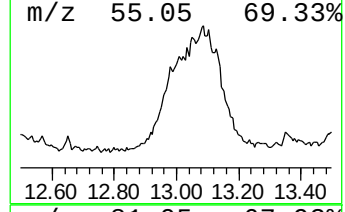
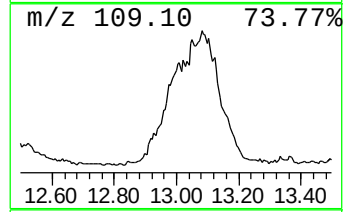
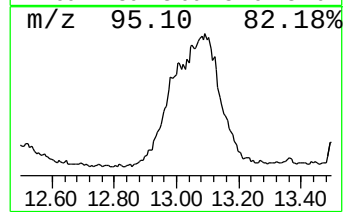
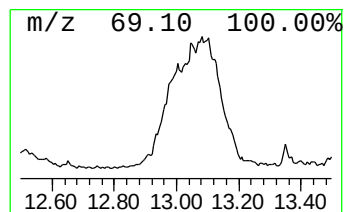
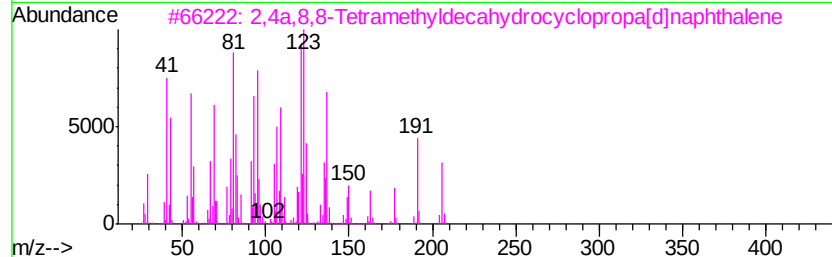
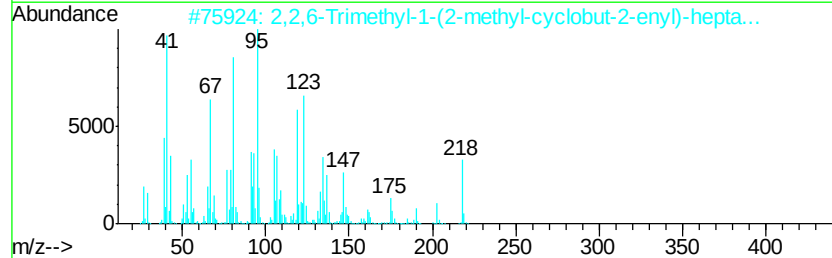
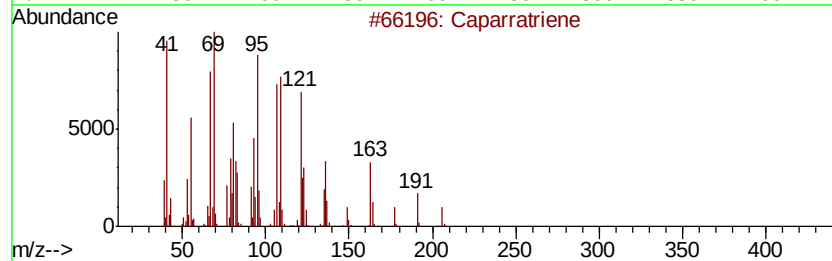
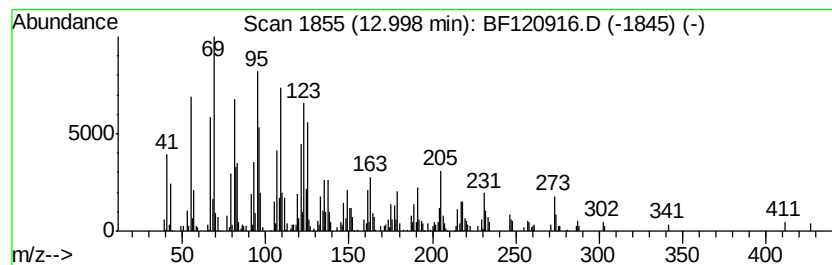
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Peak Number 2 Caparratriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	11.33 ng	802673	Chrysene-d12	13.97
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Caparratriene	206 C15H26	1000374-08-7	64
2	2,2,6-Trimethyl-1-(2-methyl-cycl...	218 C15H22O	1000188-72-8	60
3	2,4a,8,8-Tetramethyldecahydrocyc...	206 C15H26	074022-04-1	46
4	1H-Imidazole, 2-ethyl-	96 C5H8N2	001072-62-4	38
5	Germacre-1(10),4,11(13)-trien-12...	232 C15H20O2	000553-21-9	27



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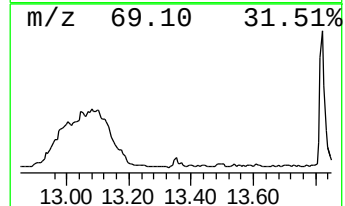
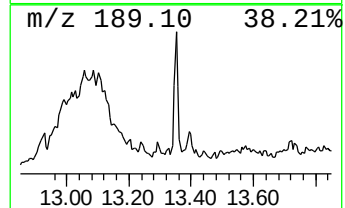
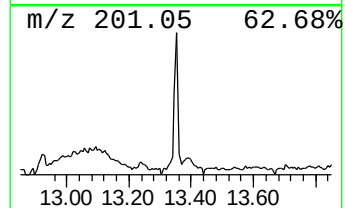
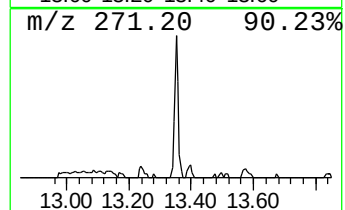
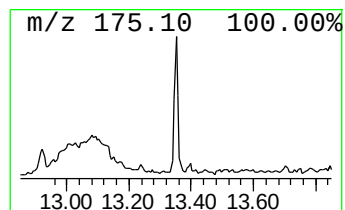
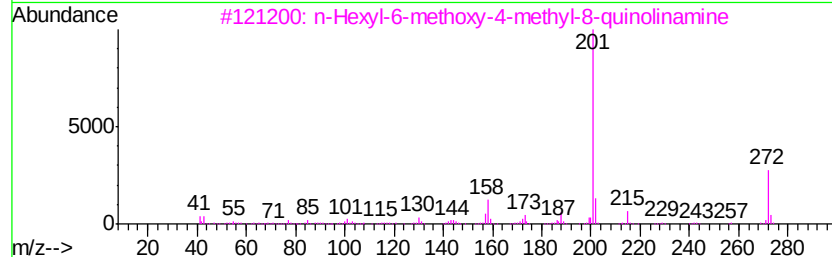
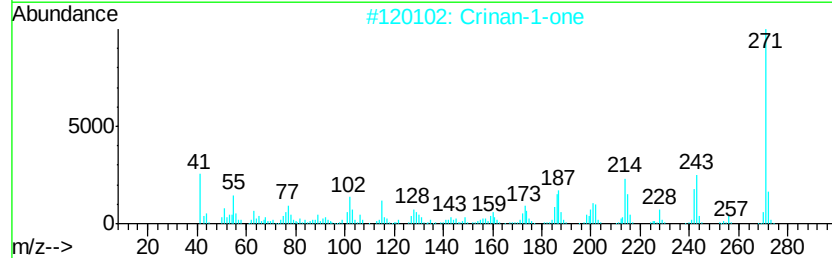
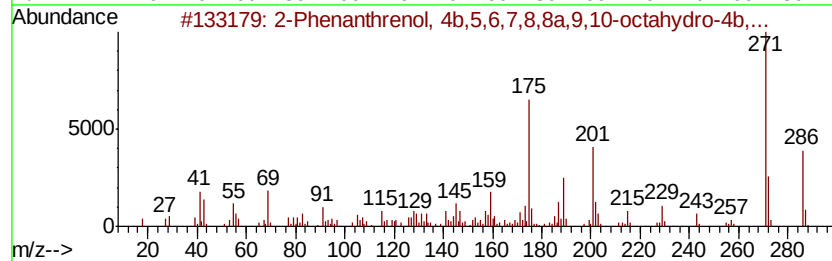
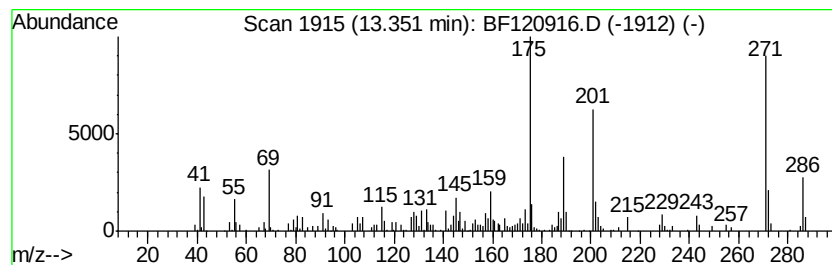
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Peak Number 3 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.35	2.30 ng	163166	Chrysene-d12	13.97		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	91	
2	Crinan-1-one	271	C16H17NO3	098301-98-5	22	
3	n-Hexyl-6-methoxy-4-methyl-8-qui...	272	C17H24N2O	083547-16-4	15	
4	Morphinan-6-ol, 4,5-epoxy-N-meth...	271	C17H21NO2	083475-40-5	14	
5	2-(1-Hydroxynaphthyl-2)quinoline	271	C19H13NO	024641-28-9	14	



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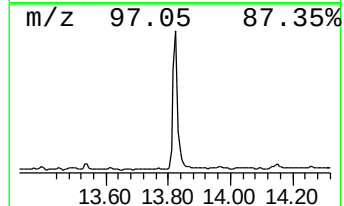
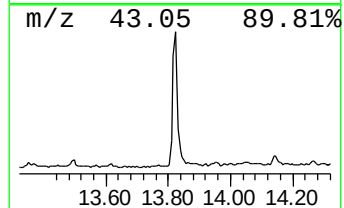
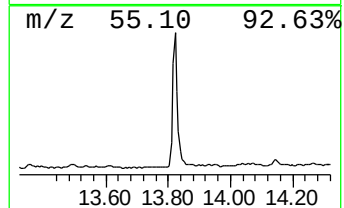
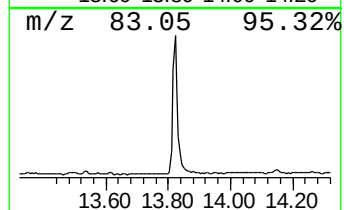
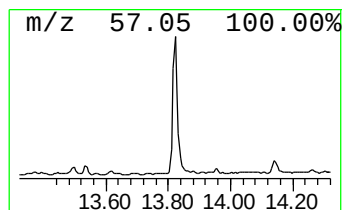
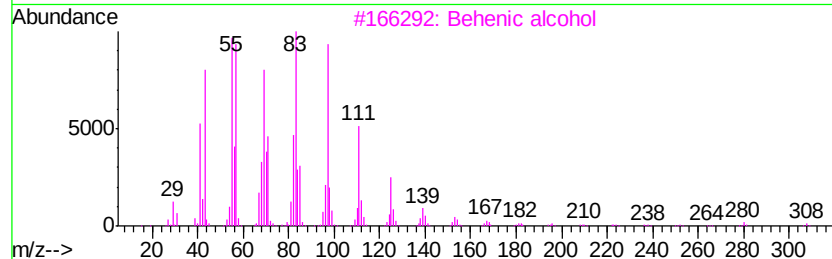
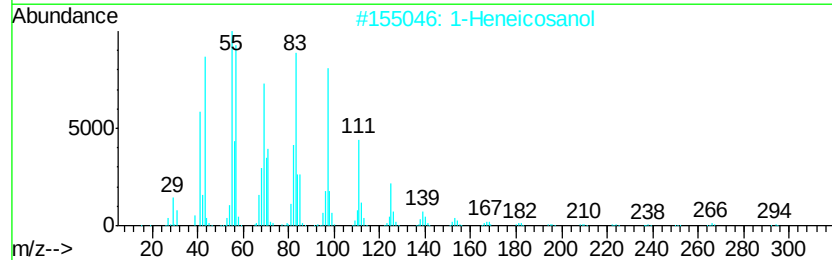
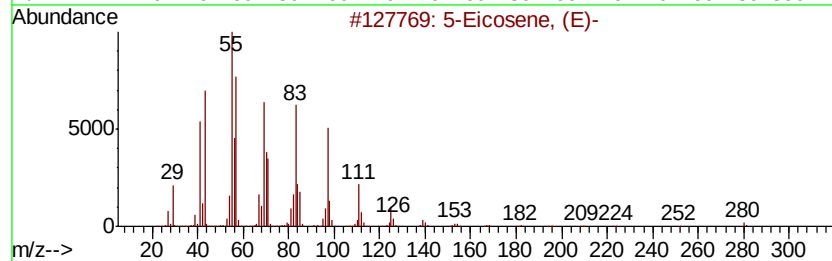
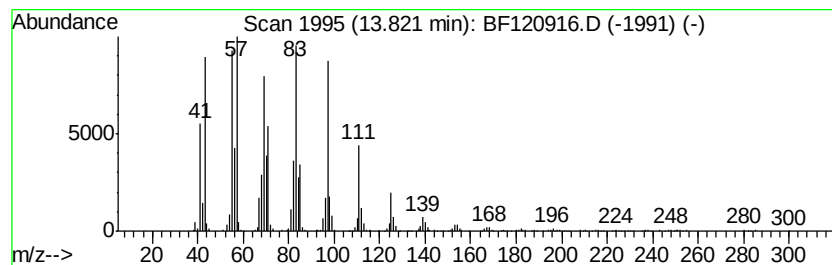
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	14.75 ng	1044930	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	1-Heneicosanol		312	C21H44O	015594-90-8	95
3	Behenic alcohol		326	C22H46O	000661-19-8	94
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	94
5	1-Heptacosanol		396	C27H56O	002004-39-9	94



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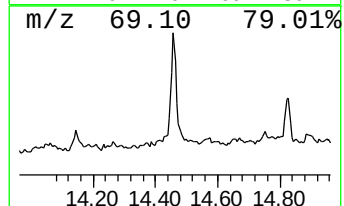
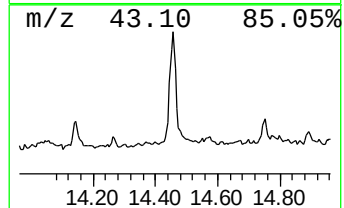
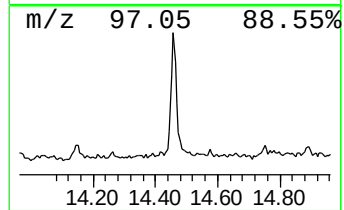
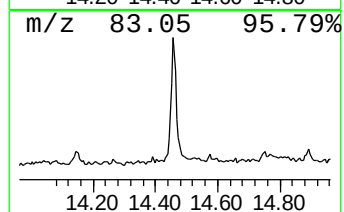
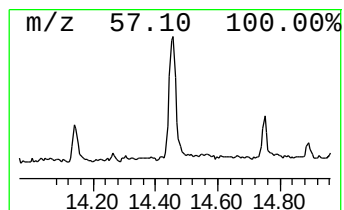
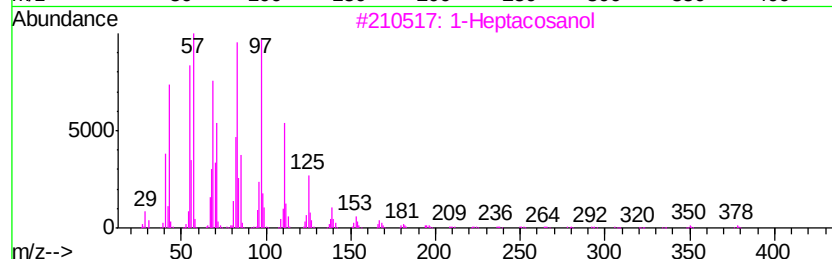
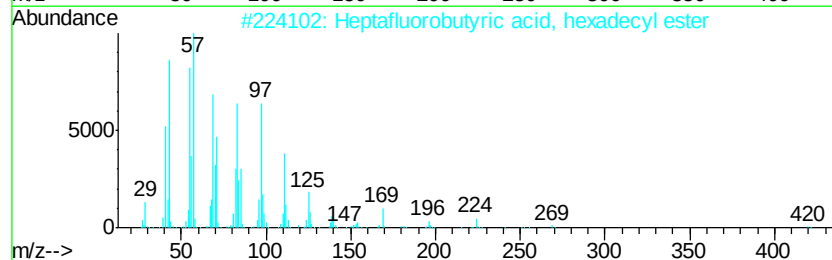
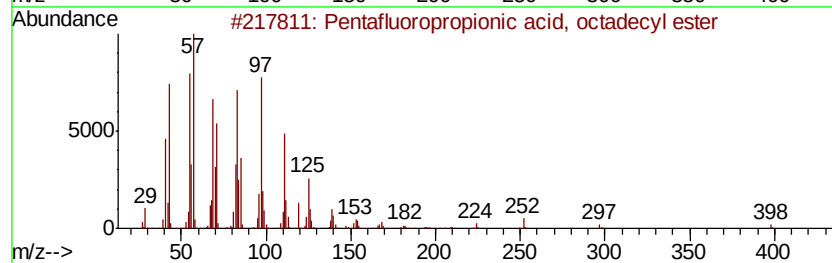
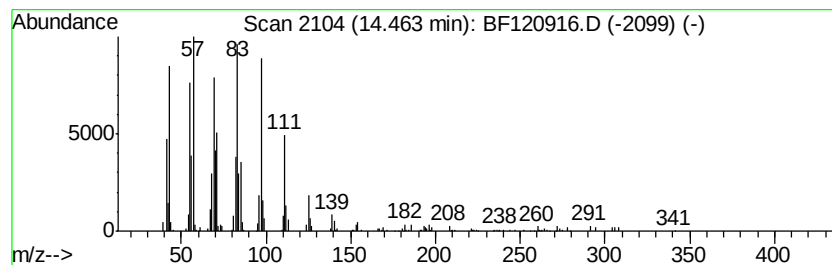
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	4.81 ng	340560	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, octadec...	416	C21H37F5O2	959261-25-7	94
2		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
3		1-Heptacosanol	396	C27H56O	002004-39-9	94
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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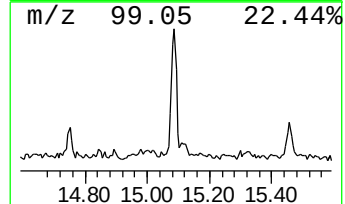
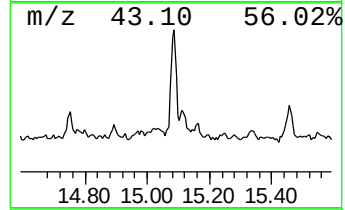
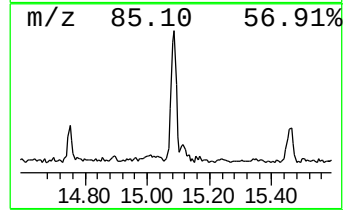
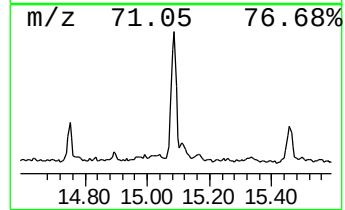
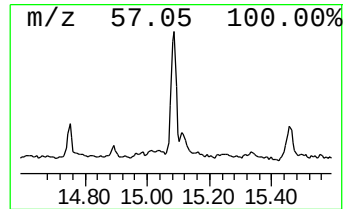
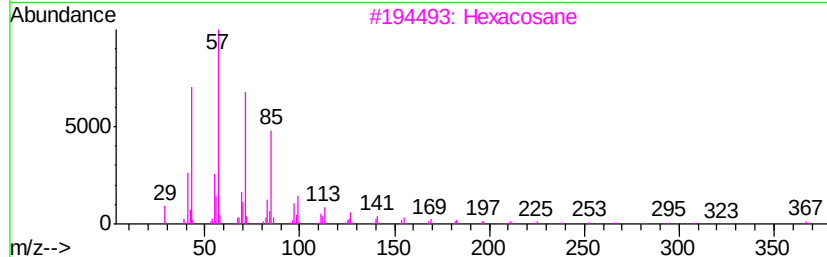
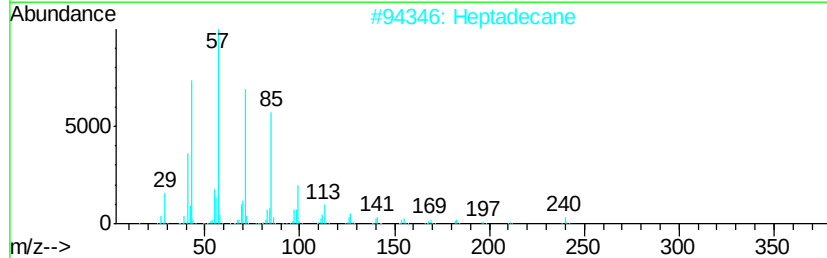
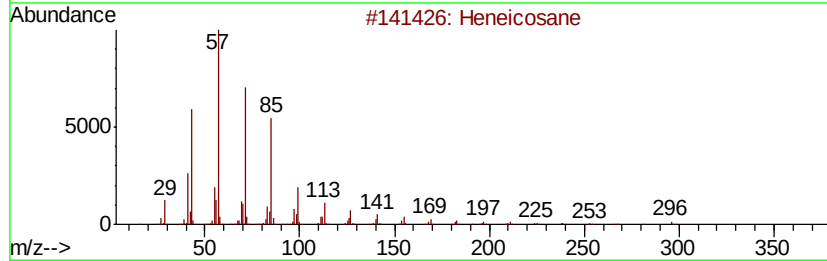
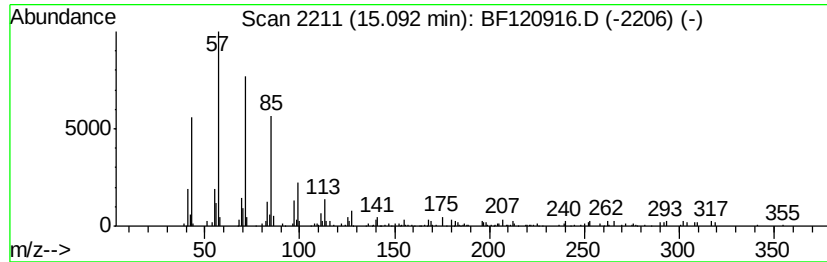
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.96 ng	173888	Perylene-d12	15.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	97
2	Heptadecane		240	C17H36	000629-78-7	94
3	Hexacosane		366	C26H54	000630-01-3	91
4	Octacosane		394	C28H58	000630-02-4	91
5	2-methyloctacosane		408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071720\
Data File : BF120916.D
Acq On : 17 Jul 2020 12:02
Operator : JU/CG
Sample : L3308-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

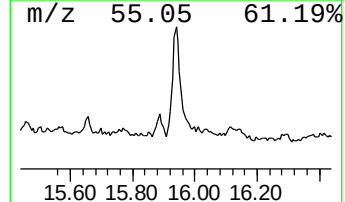
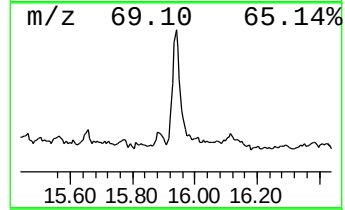
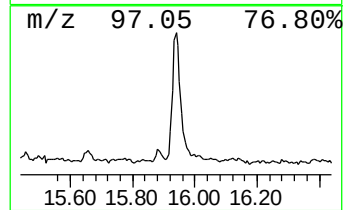
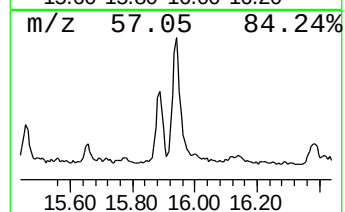
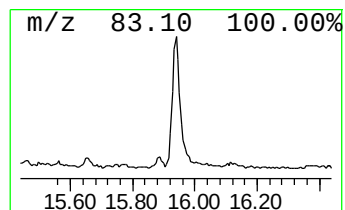
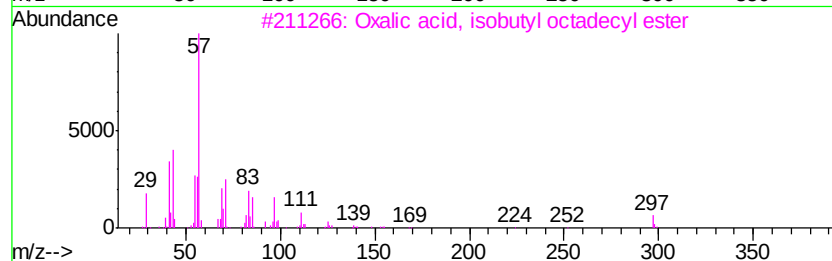
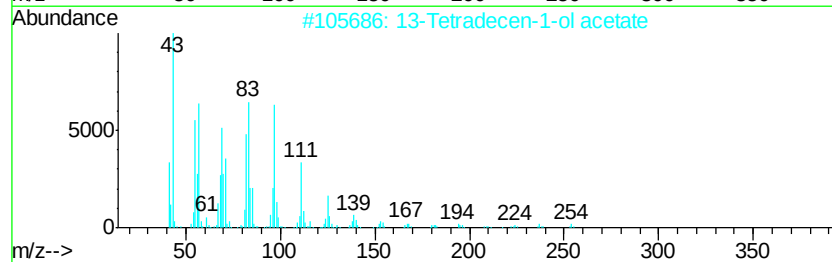
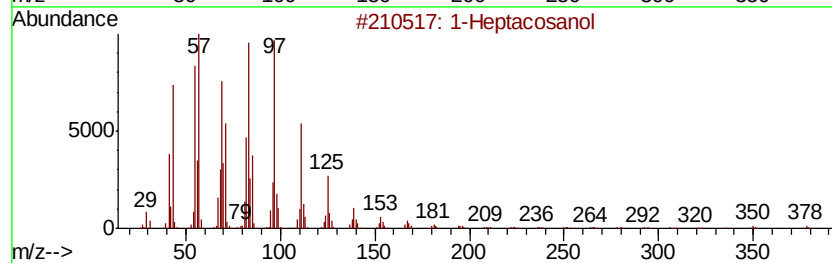
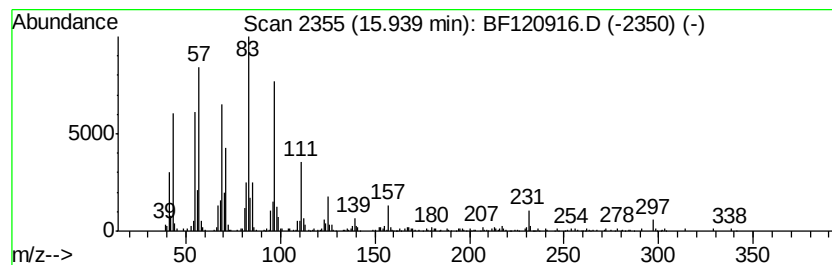
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heptacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	9.05 ng	532046	Perylene-d12	15.42
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heptacosanol	396 C27H56O	002004-39-9 93
2		13-Tetradecen-1-ol acetate	254 C16H30O2	056221-91-1 68
3		Oxalic acid, isobutyl octadecyl ...	398 C24H46O4	1000309-38-3 62
4		Octacosyl acetate	452 C30H60O2	018206-97-8 60
5		Eicosyl heptafluorobutyrate	494 C24H41F7O2	1000351-83-5 60



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071720\
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Acq On : 17 Jul 2020 12:02
Operator : JU/CG
Sample : L3308-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

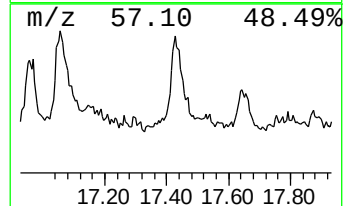
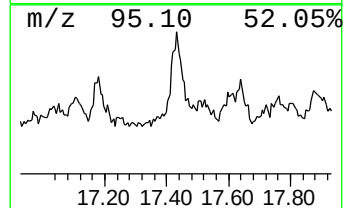
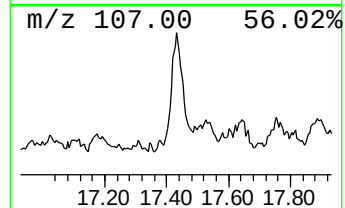
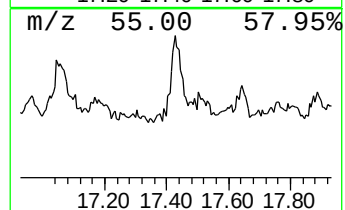
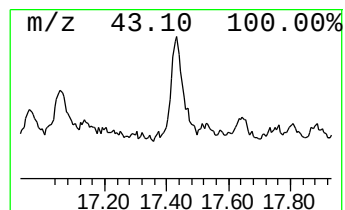
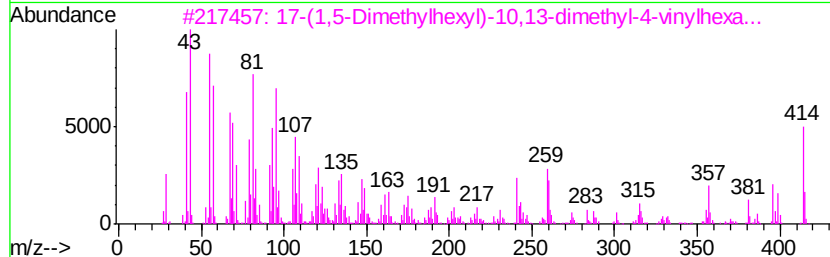
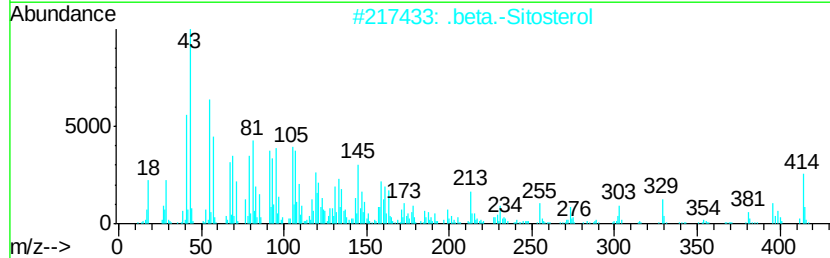
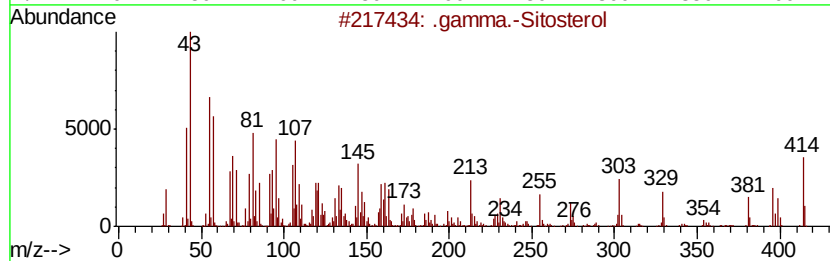
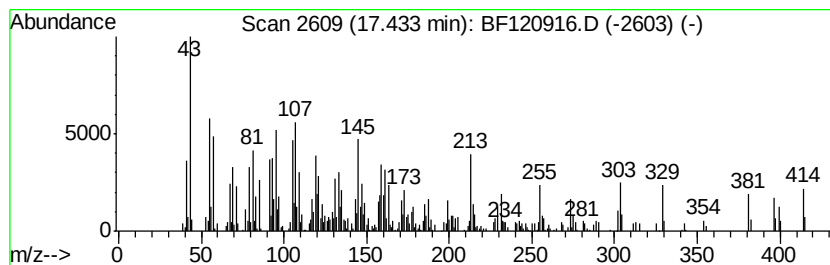
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.43	7.52 ng	441982	Perylene-d12	15.42	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	53
4	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	53
5	Campesterol	400	C28H48O	000474-62-4	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071720\
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Acq On : 17 Jul 2020 12:02
Operator : JU/CG
Sample : L3308-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

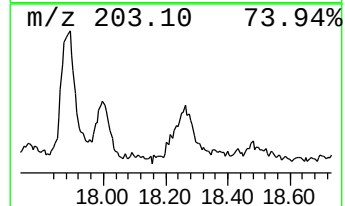
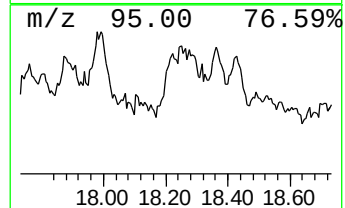
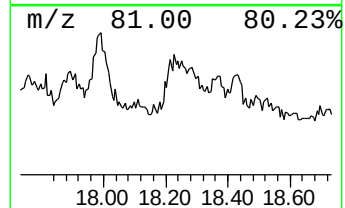
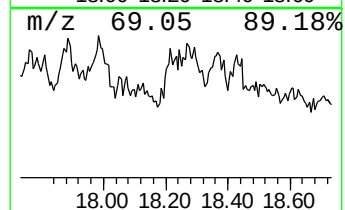
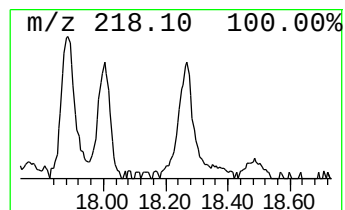
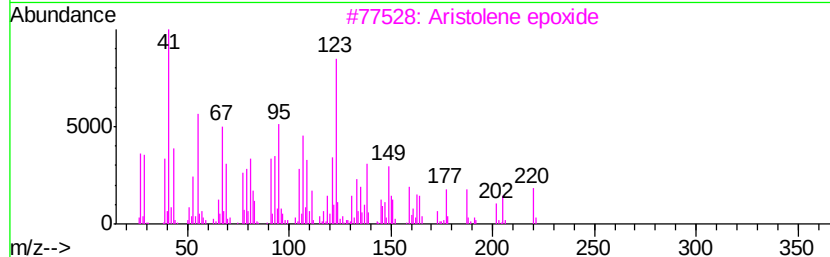
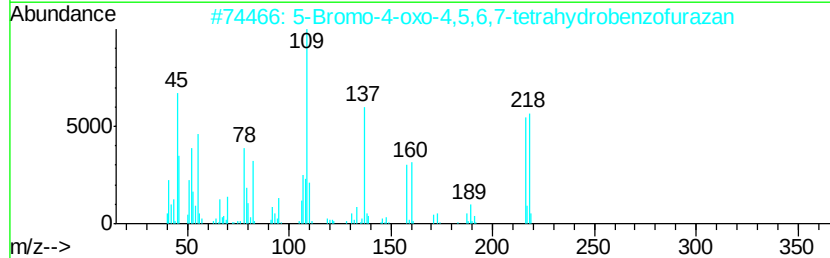
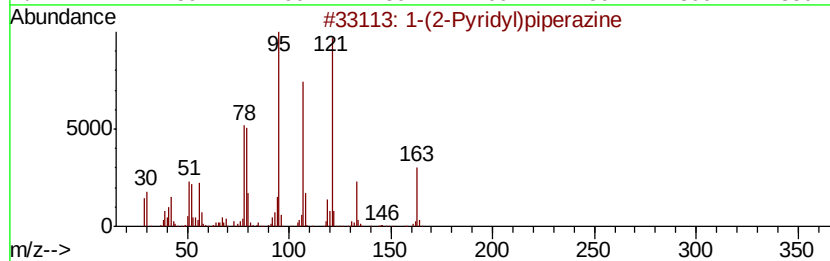
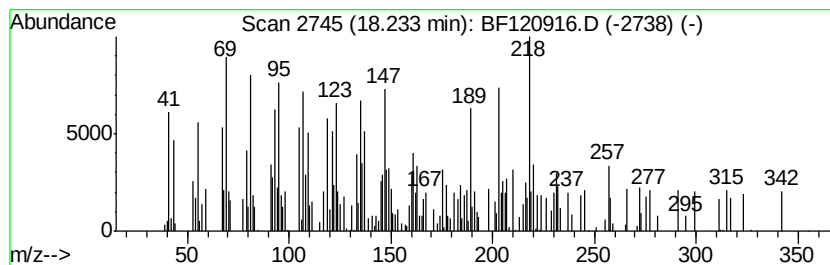
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071620.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-(2-Pyridyl)piperazine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.23	2.23 ng	131242	Perylene-d12	15.42		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	60
2		5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	53
3		Aristolene epoxide	220	C15H24O	1000151-48-9	46
4		Longipinocarveol, trans-	220	C15H24O	1000159-36-5	46
5		4,7-Methanoazulene, decahydro-1,...	206	C15H26	020478-88-0	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF071720\
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Acq On : 17 Jul 2020 12:02
Operator : JU/CG
Sample : L3308-22
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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
n-Hexadecanoic acid	11.87	2.6 ng		239905	4	11.33	1841010	20.0
Caparratriene	13.00	11.3 ng		802673	5	13.97	1417000	20.0
2-Phenanthrenol, ...	13.35	2.3 ng		163166	5	13.97	1417000	20.0
5-Eicosene, (E)-	13.82	14.8 ng		1044930	5	13.97	1417000	20.0
Pentafluoropropio...	14.46	4.8 ng		340560	5	13.97	1417000	20.0
Heneicosane	15.09	3.0 ng		173888	6	15.42	1175450	20.0
1-Heptacosanol	15.94	9.1 ng		532046	6	15.42	1175450	20.0
.gamma.-Sitosterol	17.43	7.5 ng		441982	6	15.42	1175450	20.0
1-(2-Pyridyl)pipe...	18.23	2.2 ng		131242	6	15.42	1175450	20.0