

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
 Data File : BF116740.D
 Acq On : 1 Sep 2019 14:10
 Operator : HP/JU
 Sample : K4525-19
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T9-12-13-C-(0-1.9)

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-BF083019.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	5.451	568	572	576	rBV	1578892	1404969	50.96%	5.199%
2	6.469	740	745	756	rBV	1913738	1780797	64.59%	6.590%
3	6.610	765	769	772	rBV	1948683	1626988	59.01%	6.021%
4	6.845	805	809	812	rBV	881277	724910	26.29%	2.683%
5	6.998	832	835	839	rVB	1411598	1160746	42.10%	4.295%
6	7.398	899	903	906	rBV	1351235	1086967	39.43%	4.022%
7	8.128	1023	1027	1030	rBV	1107068	983538	35.67%	3.640%
8	9.198	1205	1209	1212	rBV	2924162	2348592	85.19%	8.691%
9	9.586	1272	1275	1279	rBV	124676	90076	3.27%	0.333%
10	9.875	1321	1324	1328	rBV	1312020	1169962	42.44%	4.330%
11	10.657	1453	1457	1461	rBV	1475603	1445589	52.43%	5.350%
12	11.357	1572	1576	1579	rBV	1466590	1244378	45.13%	4.605%
13	11.380	1579	1580	1584	rVV	180489	94011	3.41%	0.348%
14	11.427	1584	1588	1593	rVB2	26913	31573	1.15%	0.117%
15	11.880	1657	1665	1677	rBV	340502	469479	17.03%	1.737%
16	12.563	1778	1781	1785	rBV	306462	278146	10.09%	1.029%
17	12.610	1787	1789	1794	rVB2	42206	36893	1.34%	0.137%
18	12.669	1794	1799	1806	rBV	600259	697275	25.29%	2.580%
19	12.763	1812	1815	1816	rBV	39536	34132	1.24%	0.126%
20	12.792	1817	1820	1823	rVB	260269	229115	8.31%	0.848%
21	12.939	1841	1845	1848	rBV	3059173	2757016	100.00%	10.203%
22	13.121	1869	1876	1879	rBV2	40921	67439	2.45%	0.250%
23	13.169	1879	1884	1885	rBV5	23044	37997	1.38%	0.141%
24	13.321	1907	1910	1913	rBV2	33608	35805	1.30%	0.132%
25	13.416	1923	1926	1931	rVB	215590	185170	6.72%	0.685%
26	13.739	1970	1981	1982	rBV4	58879	122100	4.43%	0.452%
27	13.833	1994	1997	2007	rVB3	283266	385743	13.99%	1.427%
28	13.986	2018	2023	2026	rBV	1401308	1387483	50.33%	5.134%
29	14.010	2026	2027	2033	rVB	144776	93568	3.39%	0.346%
30	14.157	2048	2052	2057	rVB	130795	124471	4.51%	0.461%
31	14.333	2074	2082	2091	rBV3	86614	223240	8.10%	0.826%
32	14.463	2099	2104	2108	rBV	247807	272140	9.87%	1.007%
33	14.763	2150	2155	2166	rBV	428176	519500	18.84%	1.922%
34	14.839	2166	2168	2174	rVB3	23195	30896	1.12%	0.114%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.015	2193	2198	2201	rBV	115334	179634	6.52%	0.665%
36	15.098	2207	2212	2218	rVB	475251	547600	19.86%	2.026%
37	15.310	2245	2248	2254	rVB	59552	79789	2.89%	0.295%
38	15.374	2254	2259	2262	rVV	86852	104155	3.78%	0.385%
39	15.439	2264	2270	2273	rVV	1003669	1231479	44.67%	4.557%
40	15.474	2273	2276	2283	rVB	445181	553783	20.09%	2.049%
41	15.786	2326	2329	2336	rVB5	22493	47337	1.72%	0.175%
42	15.904	2343	2349	2354	rBV	274392	419035	15.20%	1.551%
43	15.962	2355	2359	2370	rVB	28001	83043	3.01%	0.307%
44	16.404	2428	2434	2445	rBV	141249	256878	9.32%	0.951%
45	16.868	2508	2513	2521	rVB3	39434	86242	3.13%	0.319%
46	16.986	2527	2533	2541	rBV2	50721	116741	4.23%	0.432%
47	17.156	2558	2562	2569	rVB10	15515	33058	1.20%	0.122%
48	17.304	2582	2587	2591	rBV	25033	42521	1.54%	0.157%
49	17.680	2645	2651	2661	rVB8	24775	60839	2.21%	0.225%

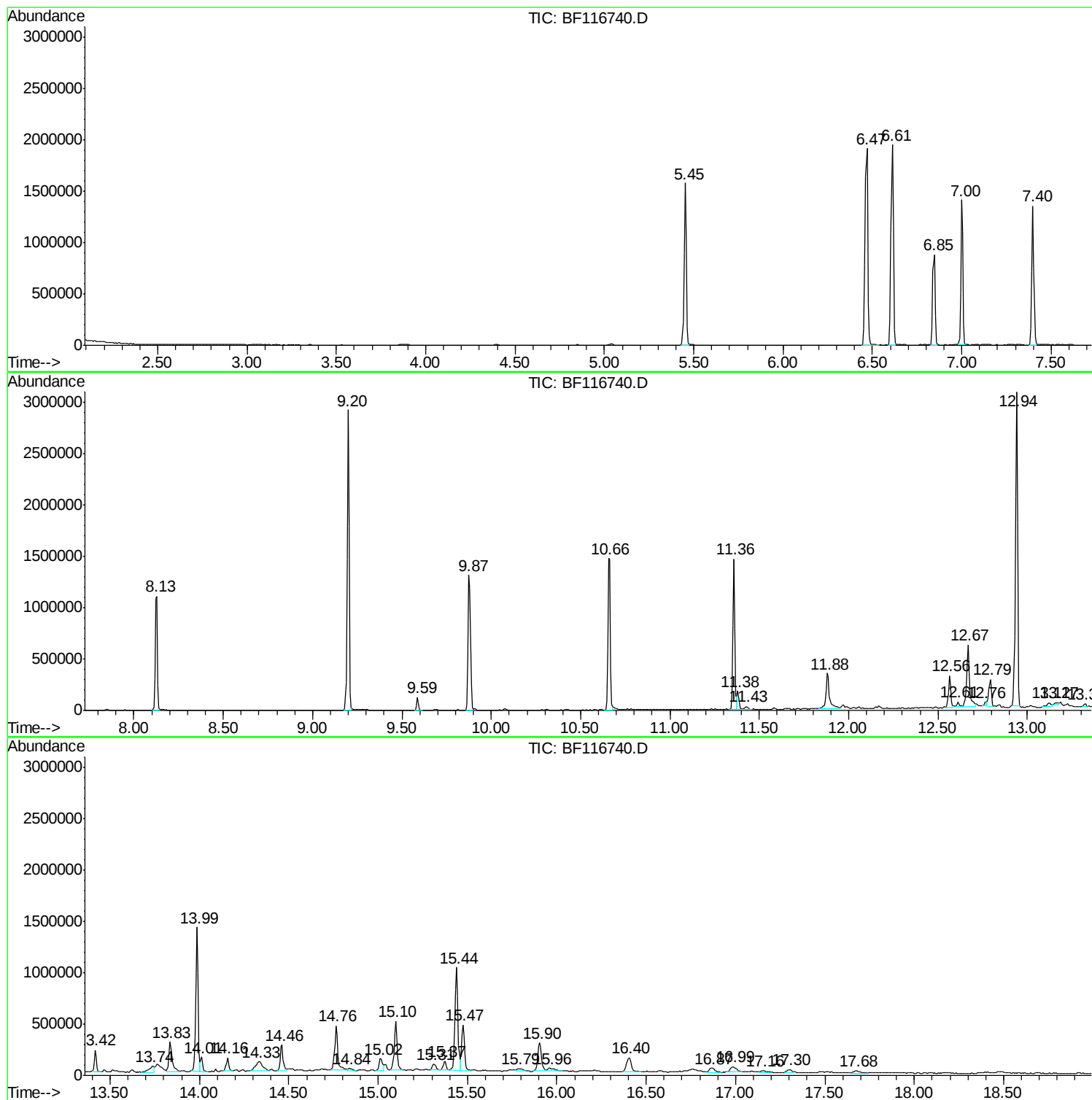
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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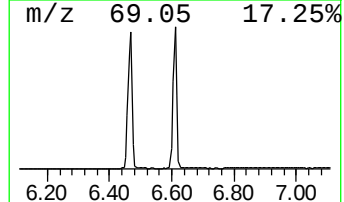
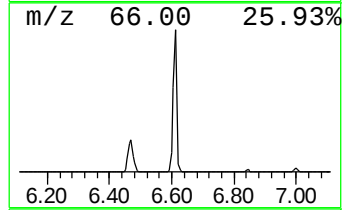
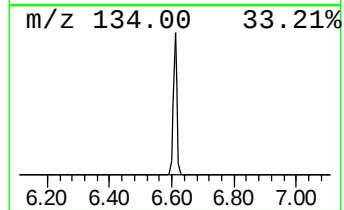
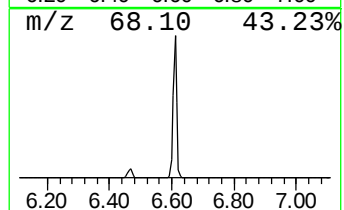
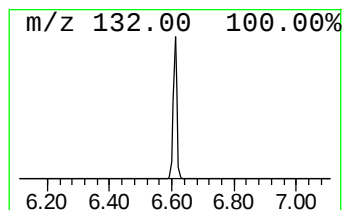
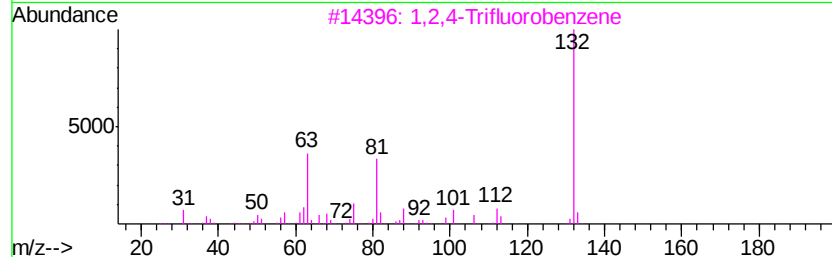
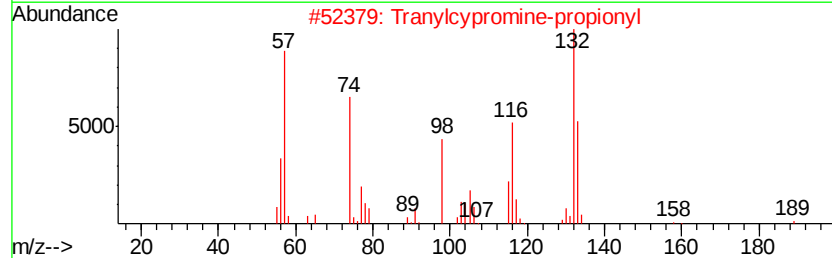
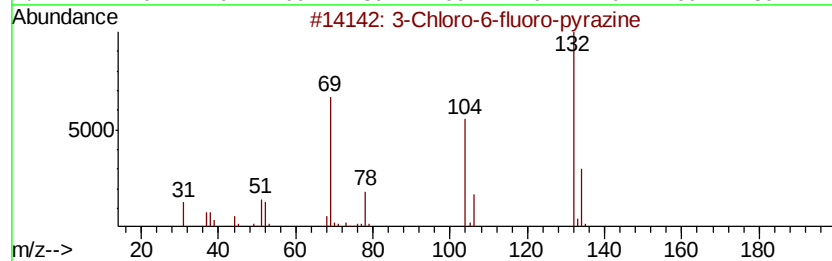
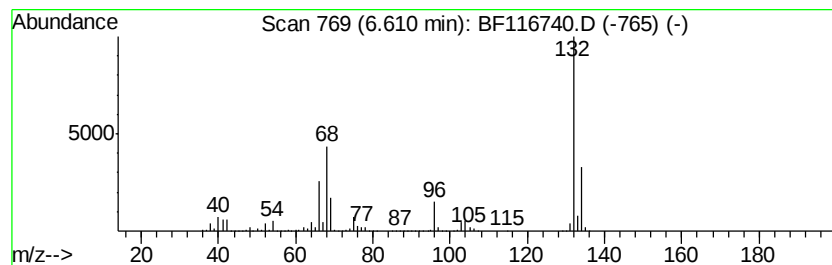
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	44.89 ng	1626990	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		Xenon	132	Xe	007440-63-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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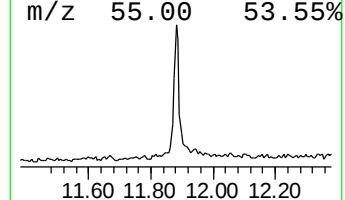
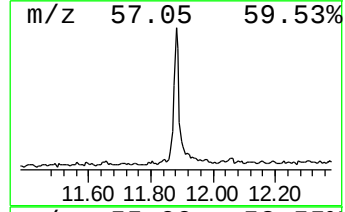
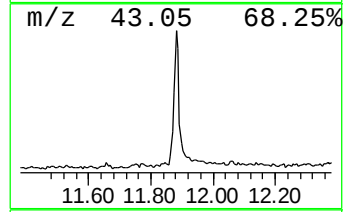
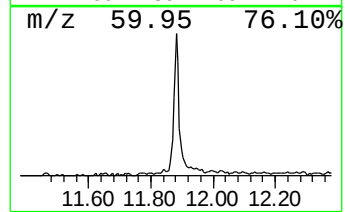
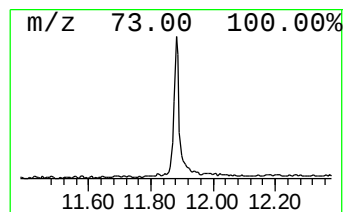
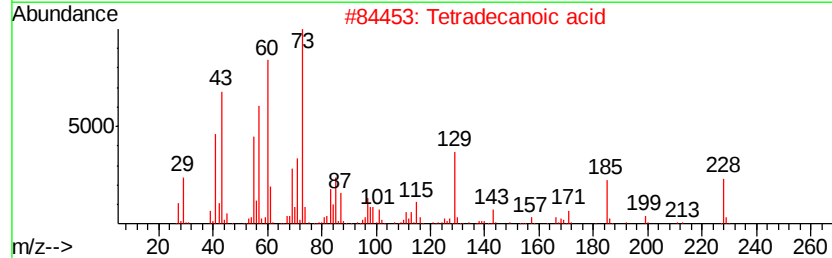
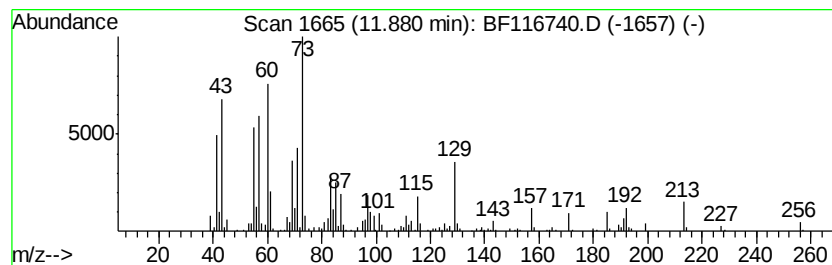
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	7.55 ng	469479	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Nonanoic acid	158	C9H18O2	000112-05-0	38



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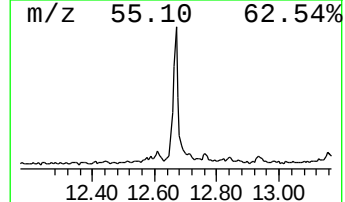
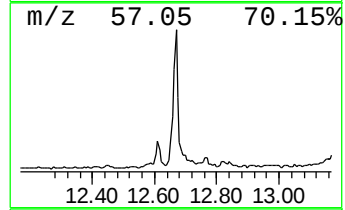
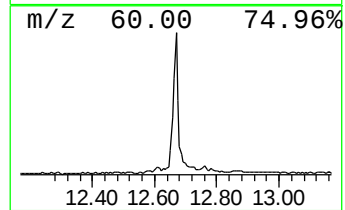
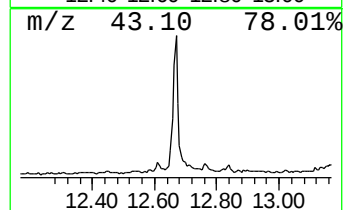
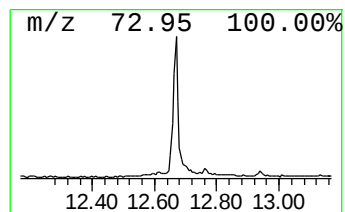
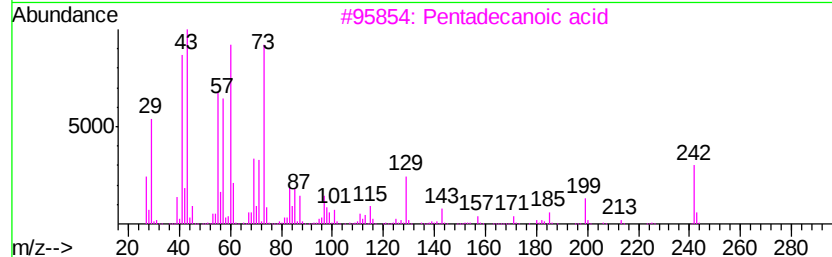
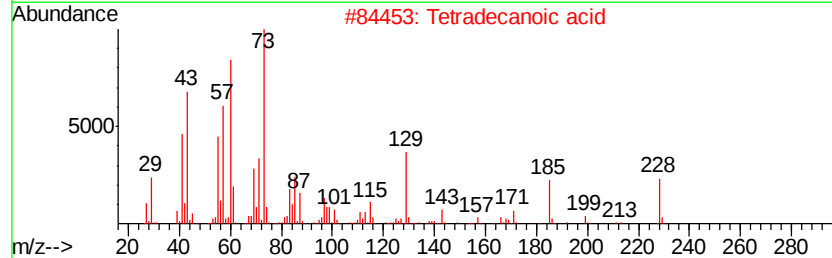
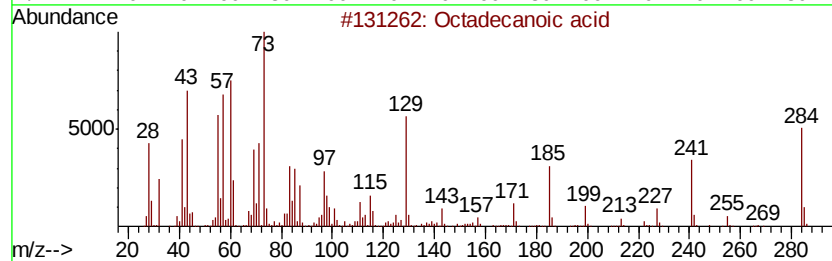
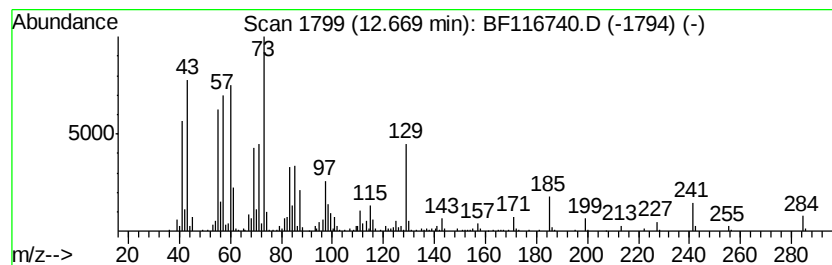
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	11.21 ng	697275	Phenanthrene-d10	11.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		n-Decanoic acid	172	C10H20O2	000334-48-5	68
5		n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25



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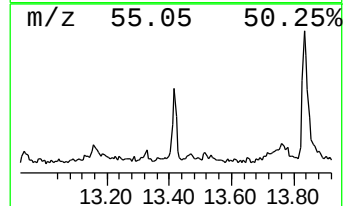
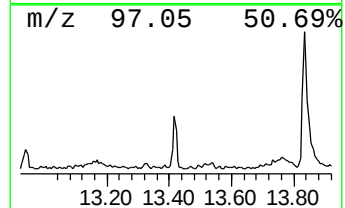
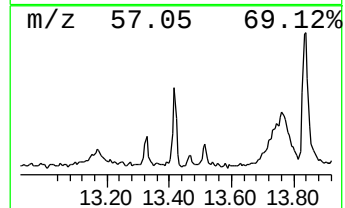
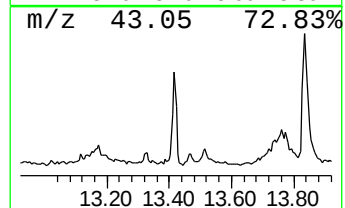
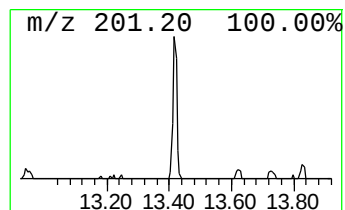
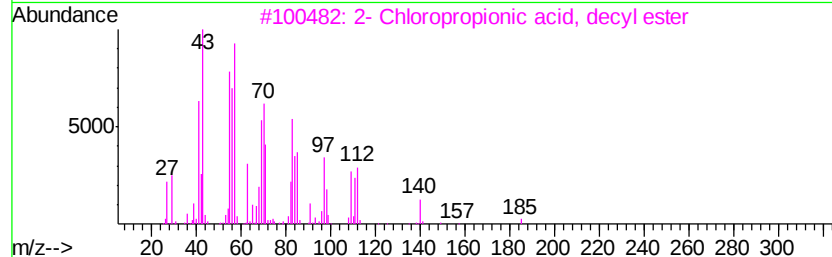
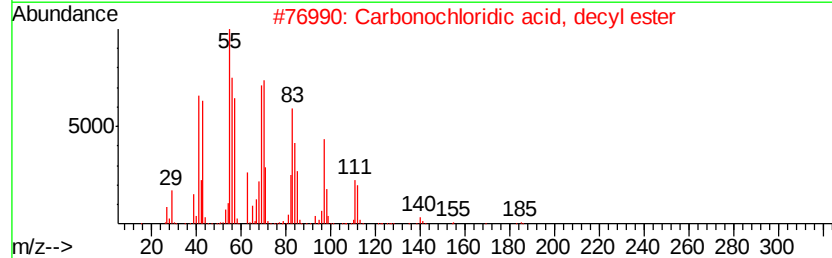
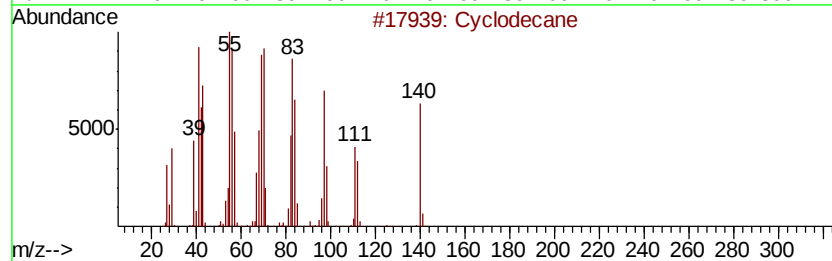
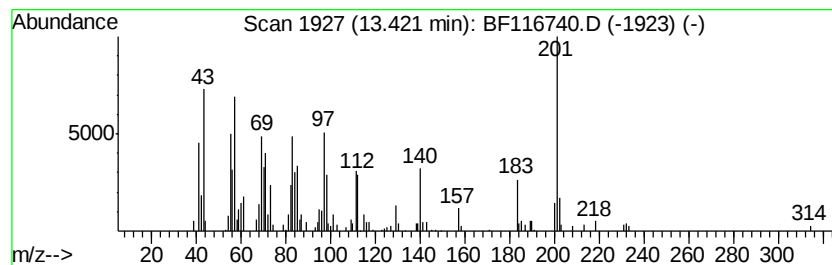
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclodecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	2.67 ng	185170	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclodecane	140	C10H20	000293-96-9	70
2		Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	46
3		2- Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	43
4		Dichloroacetic acid, dodecyl ester	296	C14H26Cl2O2	083005-01-0	43
5		1-Dodecanethiol	202	C12H26S	000112-55-0	41



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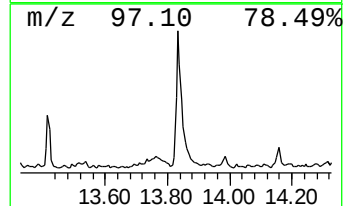
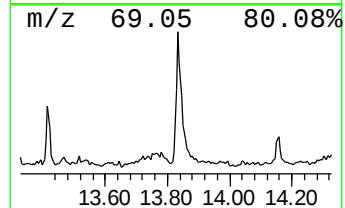
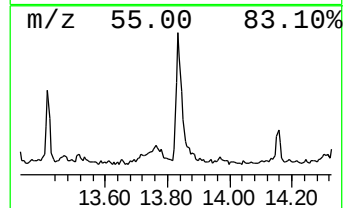
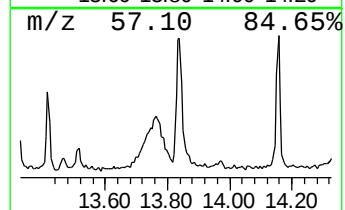
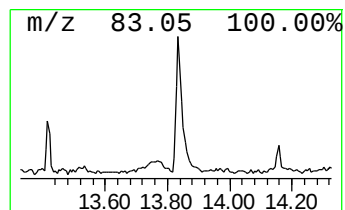
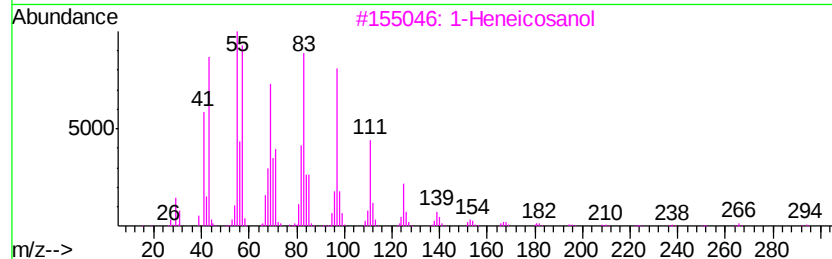
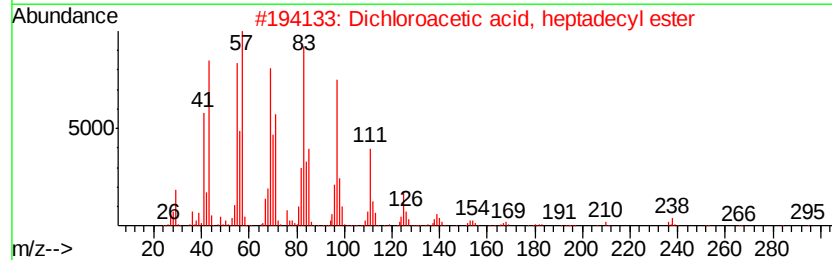
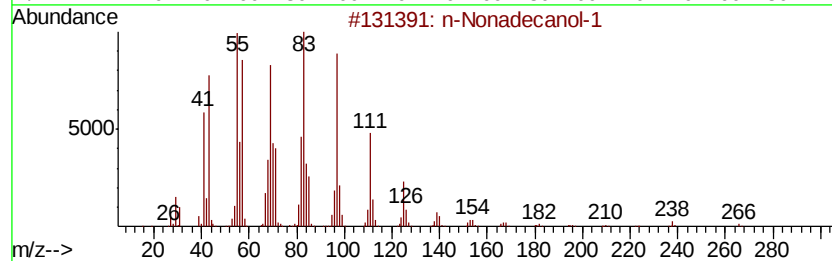
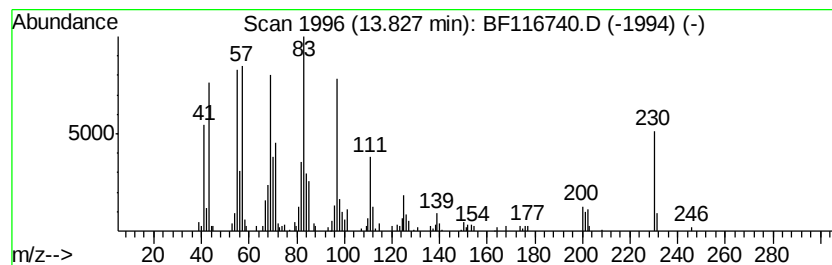
Instrument :
BNA_F
ClientSampleId :
T9-12-13-C-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Nonadecanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.83	5.56 ng	385743	Chrysene-d12	13.99		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1		284	C19H40O	001454-84-8	93
2	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	93
3	1-Heneicosanol		312	C21H44O	015594-90-8	93
4	n-Tetracosanol-1		354	C24H50O	000506-51-4	91
5	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116740.D
Acq On : 1 Sep 2019 14:10
Operator : HP/JU
Sample : K4525-19
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T9-12-13-C-(0-1.9)

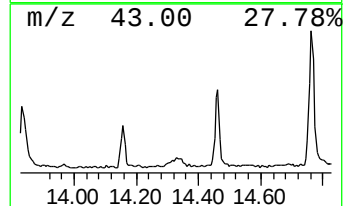
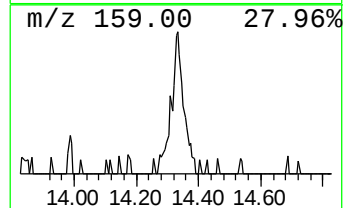
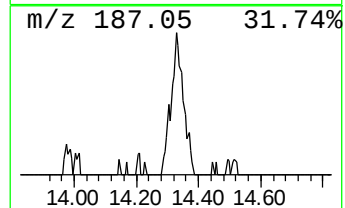
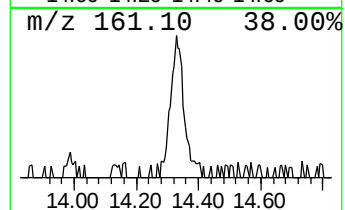
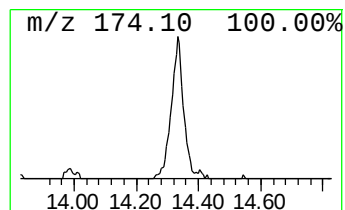
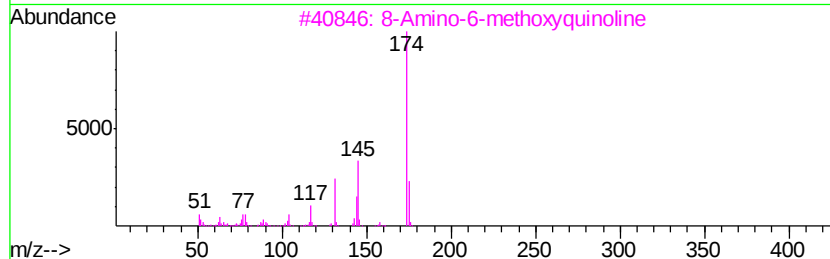
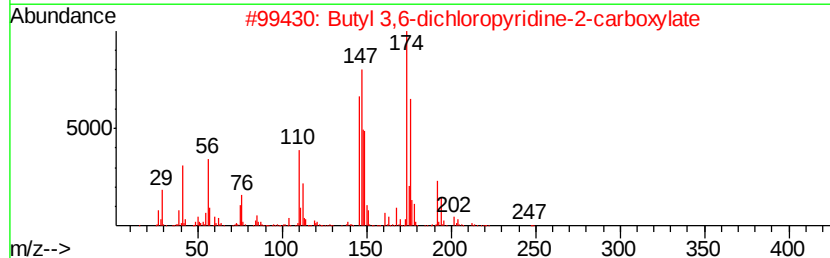
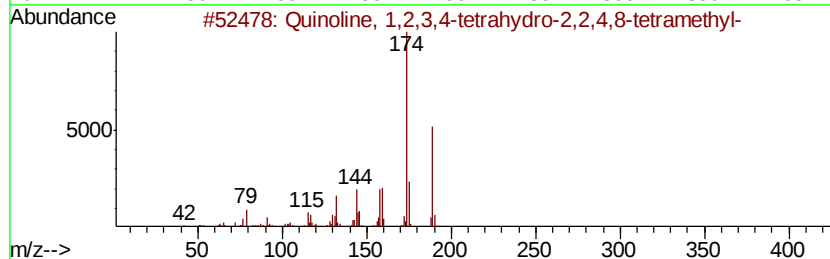
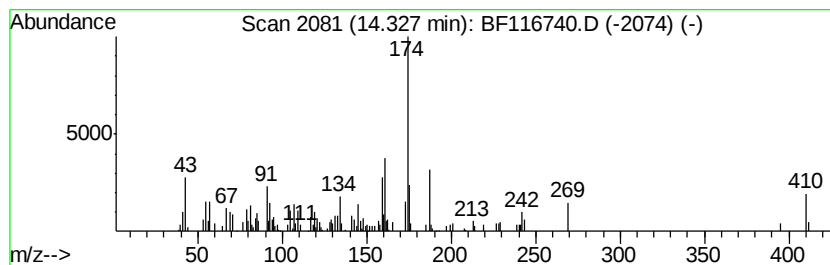
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.33 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.33	3.22 ng	223240	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Quinoline, 1,2,3,4-tetrahydro-2,...	189	C13H19N	1000308-78-8	37
2		Butyl 3,6-dichloropyridine-2-car...	247	C10H11Cl2N02	1000373-31-6	35
3		8-Amino-6-methoxyquinoline	174	C10H10N2O	000090-52-8	35
4		2-(3-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-16-1	30
5		2-(4-Fluorophenyl)pyrimidine	174	C10H7FN2	068049-17-2	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
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 Sample : K4525-19
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Instrument :
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 ClientSampleId :
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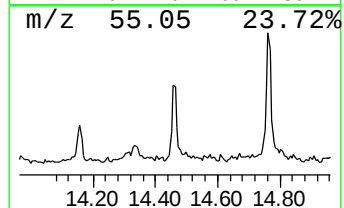
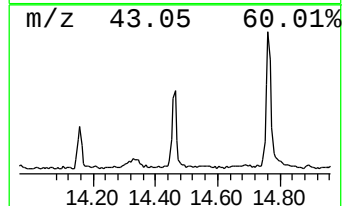
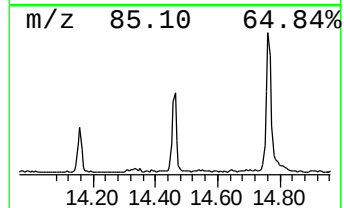
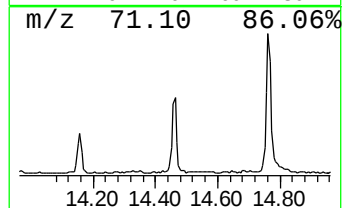
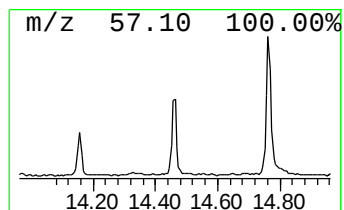
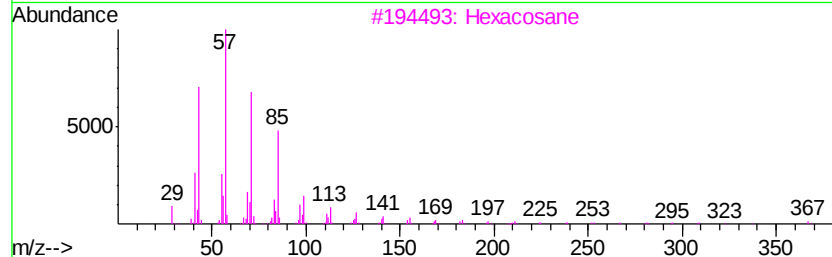
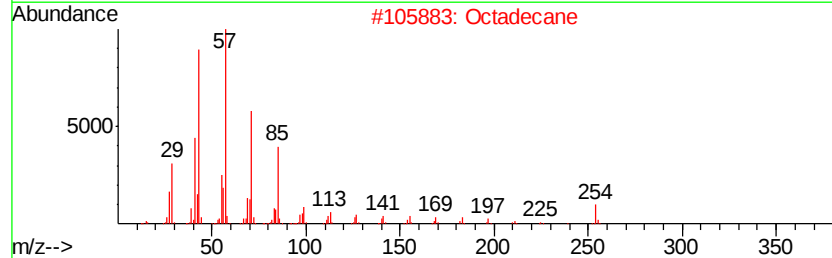
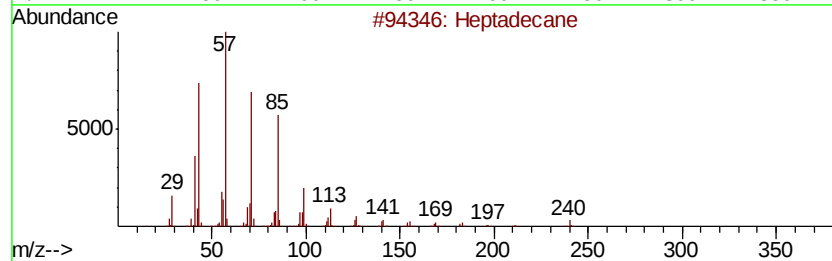
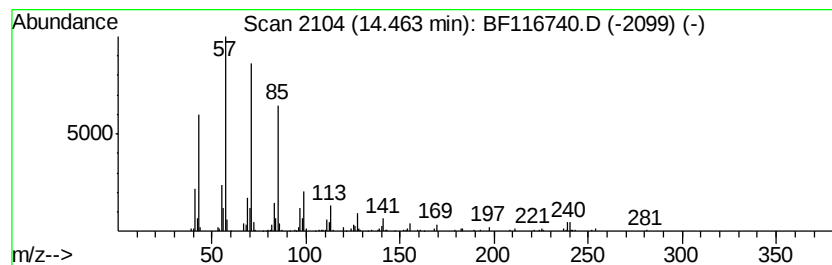
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 8 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	3.92 ng	272140	Chrysene-d12	13.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	98
2		Octadecane	254	C18H38	000593-45-3	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heneicosane	296	C21H44	000629-94-7	90
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116740.D
Acq On : 1 Sep 2019 14:10
Operator : HP/JU
Sample : K4525-19
Misc :
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Instrument :
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ClientSampleId :
T9-12-13-C-(0-1.9)

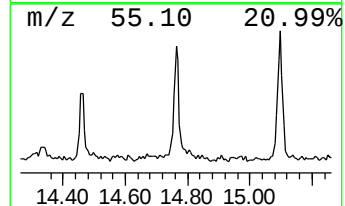
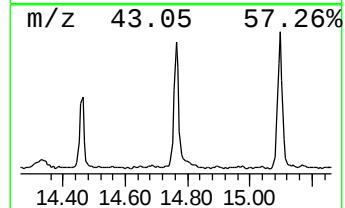
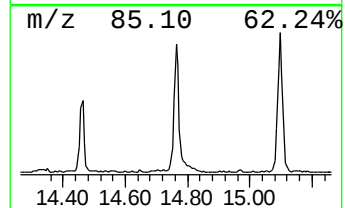
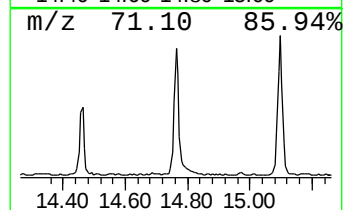
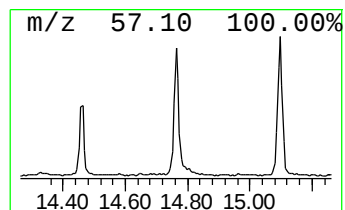
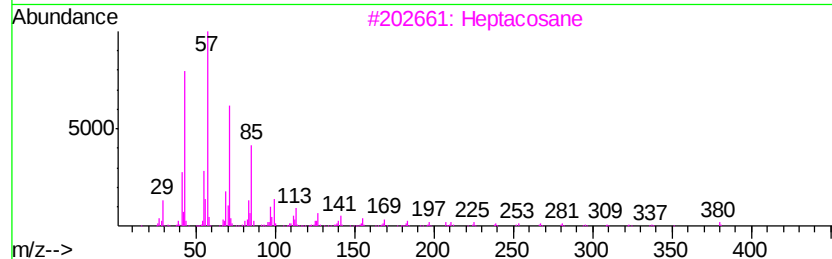
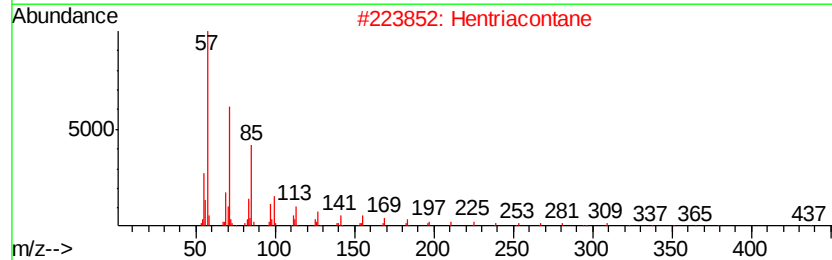
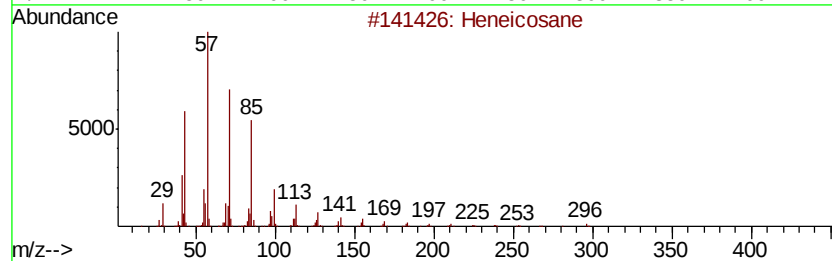
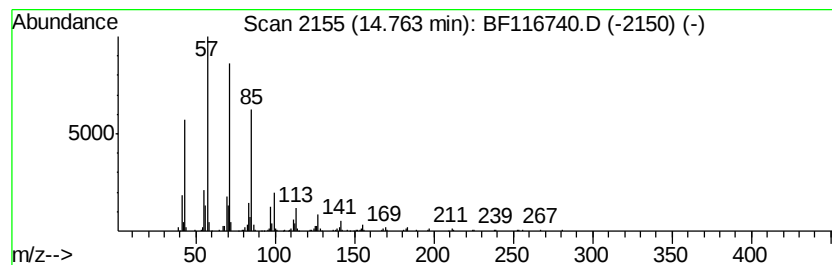
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	8.44 ng	519500	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Hentriacontane		437	C31H64	000630-04-6	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	Hexacosane		366	C26H54	000630-01-3	90
5	2-Bromotetradecane		276	C14H29Br	074036-95-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116740.D
Acq On : 1 Sep 2019 14:10
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Sample : K4525-19
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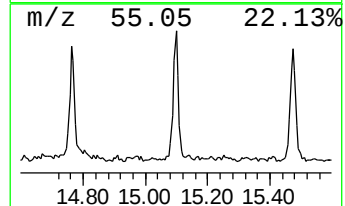
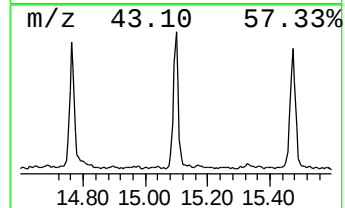
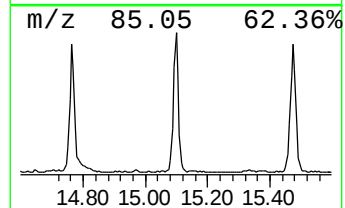
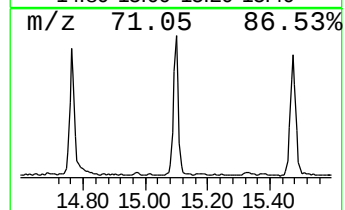
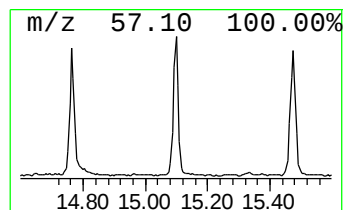
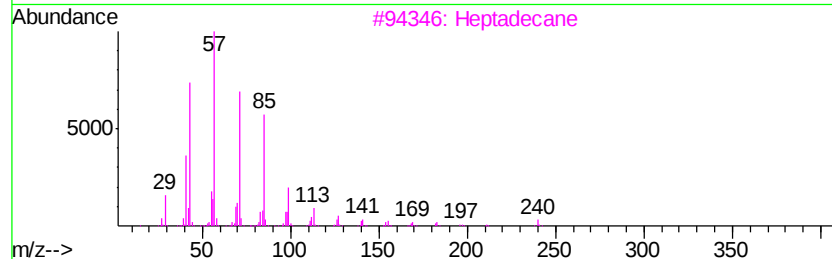
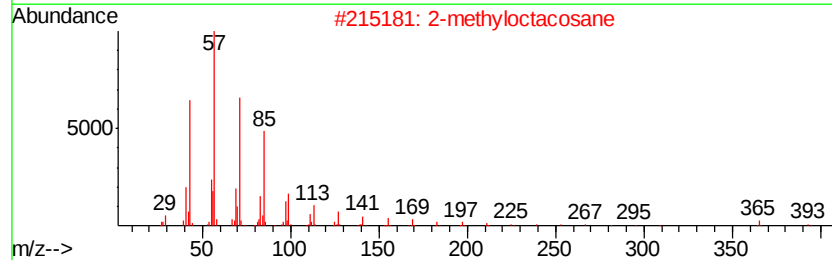
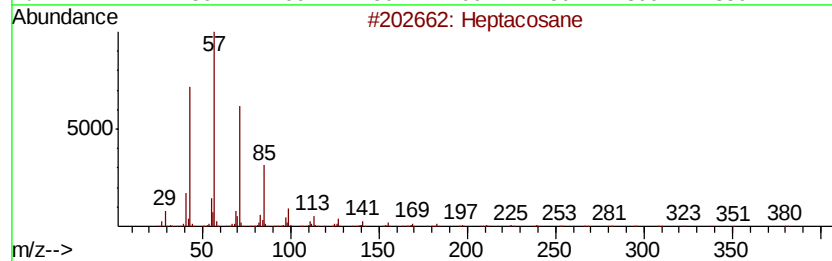
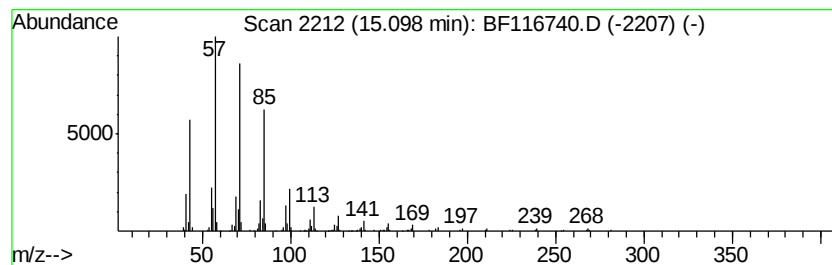
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	8.89 ng	547600	Perylene-d12	15.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	2-methyloctacosane		408	C29H60	1000376-72-8	91
3	Heptadecane		240	C17H36	000629-78-7	87
4	Docosane		310	C22H46	000629-97-0	86
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
Data File : BF116740.D
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T9-12-13-C-(0-1.9)

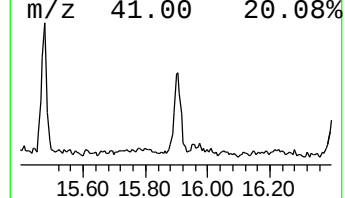
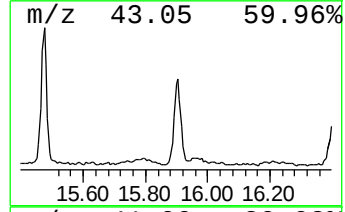
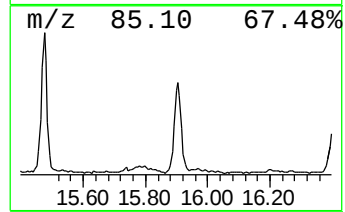
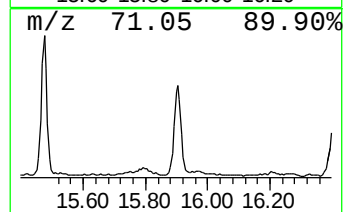
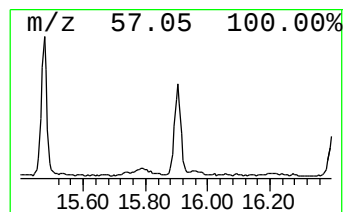
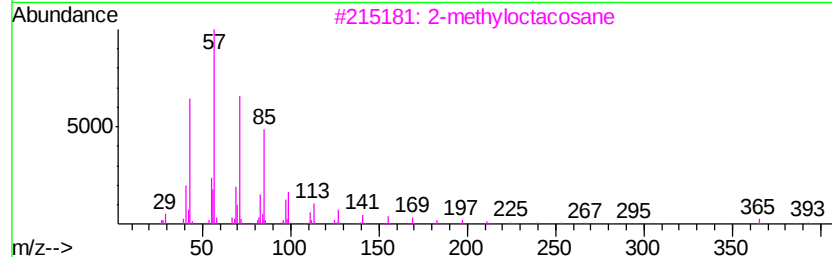
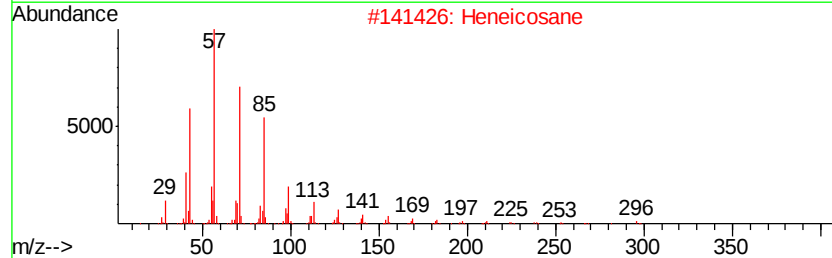
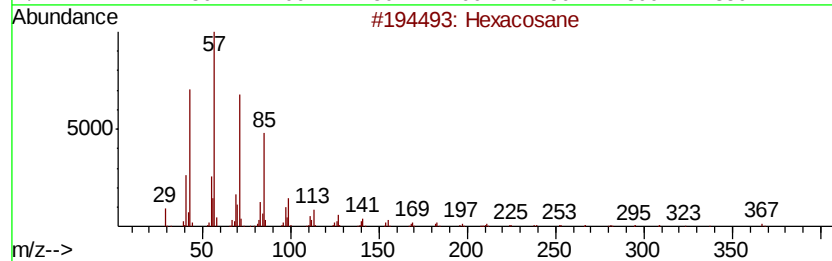
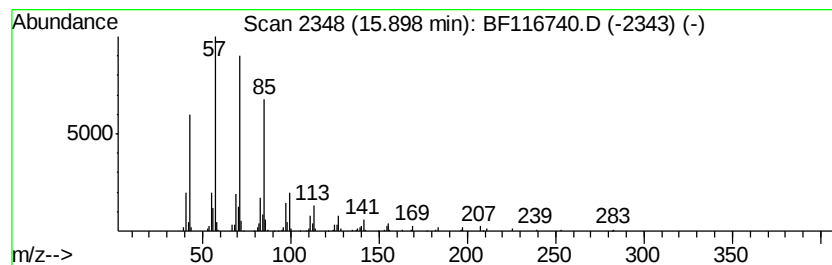
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	6.81 ng	419035	Perylene-d12	15.44

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090119\
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ALS Vial : 3 Sample Multiplier: 1

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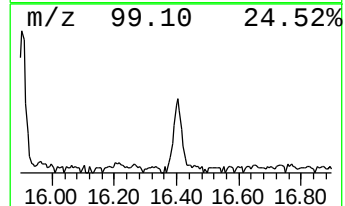
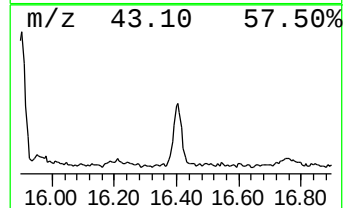
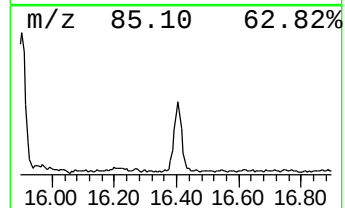
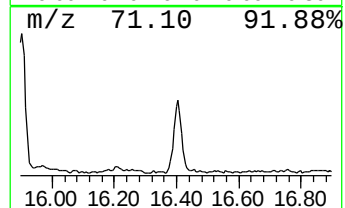
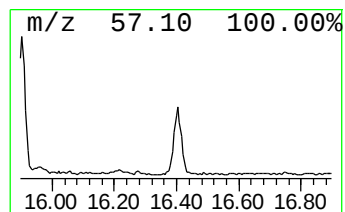
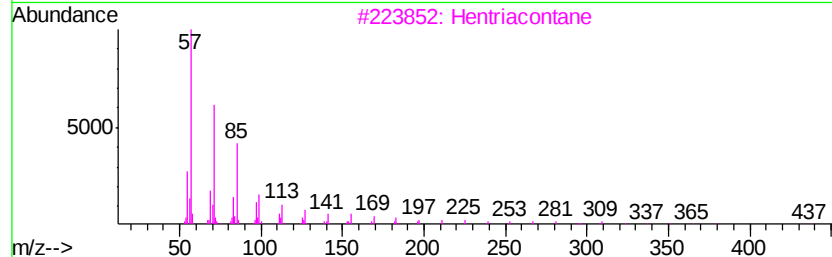
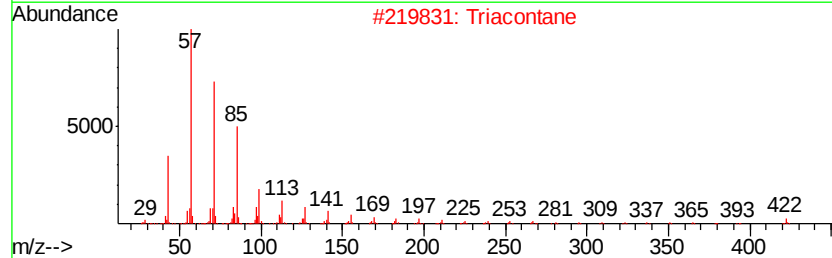
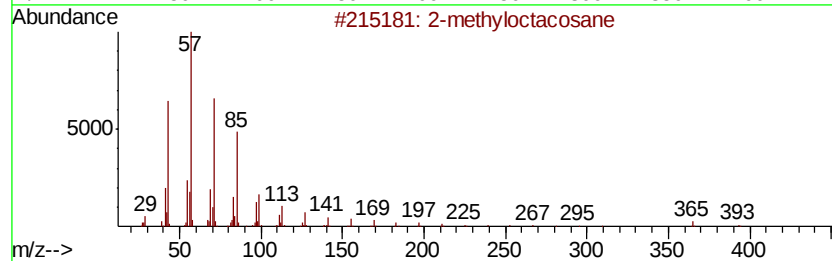
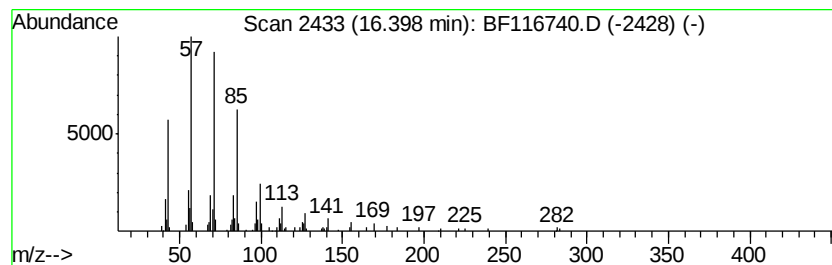
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	4.17 ng	256878	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		triacontane	422	C30H62	000638-68-6	91
3		hentriacontane	437	C31H64	000630-04-6	91
4		heneicosane	296	C21H44	000629-94-7	91
5		hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090119\
Data File : BF116740.D
Acq On : 1 Sep 2019 14:10
Operator : HP/JU
Sample : K4525-19
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T9-12-13-C-(0-1.9)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
unknown6.61	6.61	44.9	ng	1626990	1	6.85	724910	20.0
n-Hexadecanoic acid	11.88	7.5	ng	469479	4	11.36	1244380	20.0
Octadecanoic acid	12.67	11.2	ng	697275	4	11.36	1244380	20.0
Cyclodecane	13.42	2.7	ng	185170	5	13.99	1387480	20.0
n-Nonadecanol-1	13.83	5.6	ng	385743	5	13.99	1387480	20.0
unknown14.33	14.33	3.2	ng	223240	5	13.99	1387480	20.0
Heptadecane	14.46	3.9	ng	272140	5	13.99	1387480	20.0
Heneicosane	14.76	8.4	ng	519500	6	15.44	1231480	20.0
Heptacosane	15.10	8.9	ng	547600	6	15.44	1231480	20.0
Hexacosane	15.90	6.8	ng	419035	6	15.44	1231480	20.0
2-methyloctacosane	16.40	4.2	ng	256878	6	15.44	1231480	20.0