

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
 Data File : BF115436.D
 Acq On : 9 Jul 2019 16:17
 Operator : HP/JU
 Sample : K3687-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12017-VNJ-206

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-BF070519.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	2.216	16	22	34	rVB	1369786	1897568	44.82%	4.066%
2	5.516	578	583	586	rBV	3050552	3067733	72.46%	6.573%
3	6.522	748	754	757	rBV	2964863	3236057	76.43%	6.934%
4	6.663	773	778	781	rBV	3430822	3340329	78.90%	7.157%
5	6.893	814	817	821	rVB	1196519	974987	23.03%	2.089%
6	7.051	840	844	847	rBV	3029573	2610473	61.66%	5.593%
7	7.451	907	912	915	rBV	2292312	2110179	49.84%	4.521%
8	8.175	1031	1035	1038	rBV	1580180	1258359	29.72%	2.696%
9	9.251	1213	1218	1221	rBV	4301213	3768538	89.01%	8.074%
10	9.639	1280	1284	1295	rBV	1196582	935217	22.09%	2.004%
11	9.928	1329	1333	1337	rBV	1709501	1501878	35.47%	3.218%
12	10.716	1462	1467	1470	rBV	2534675	2415808	57.06%	5.176%
13	11.410	1581	1585	1588	rBV	1805188	1663666	39.30%	3.565%
14	11.945	1666	1676	1687	rBV	381911	519174	12.26%	1.112%
15	12.233	1723	1725	1731	rVB	61187	60115	1.42%	0.129%
16	12.563	1779	1781	1787	rVB2	56114	57188	1.35%	0.123%
17	12.645	1792	1795	1799	rBV	818221	779621	18.41%	1.670%
18	12.763	1809	1815	1827	rBV	787037	1052275	24.85%	2.255%
19	12.892	1830	1837	1840	rVV2	687408	845216	19.96%	1.811%
20	12.945	1843	1846	1851	rVB2	42356	56104	1.33%	0.120%
21	13.016	1854	1858	1859	rBV	51678	46883	1.11%	0.100%
22	13.051	1859	1864	1867	rVV	4255518	4233784	100.00%	9.071%
23	13.127	1871	1877	1880	rBV3	56847	88642	2.09%	0.190%
24	13.216	1889	1892	1894	rBV2	51971	61738	1.46%	0.132%
25	13.239	1894	1896	1900	rVB2	68490	74839	1.77%	0.160%
26	13.316	1904	1909	1912	rBV2	78936	92335	2.18%	0.198%
27	13.357	1912	1916	1919	rBV	94951	100652	2.38%	0.216%
28	13.804	1988	1992	1999	rVB	107615	131596	3.11%	0.282%
29	13.933	2009	2014	2018	rBV2	69971	108275	2.56%	0.232%
30	13.969	2018	2020	2022	rVV	58411	54639	1.29%	0.117%
31	13.998	2022	2025	2029	rVV2	51366	69659	1.65%	0.149%
32	14.045	2029	2033	2036	rVB2	71390	74366	1.76%	0.159%
33	14.086	2036	2040	2055	rVB4	219694	570970	13.49%	1.223%
34	14.233	2059	2065	2068	rBV	1461979	1637757	38.68%	3.509%

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72-12017-VNJ-206

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	14.257	2068	2069	2072	rVB	284625	219968	5.20%	0.471%
36	14.463	2100	2104	2108	rBV	163502	174190	4.11%	0.373%
37	14.704	2139	2145	2148	rVB	30038	46947	1.11%	0.101%
38	14.745	2148	2152	2155	rBV2	60943	71908	1.70%	0.154%
39	14.845	2165	2169	2173	rBV	358312	399512	9.44%	0.856%
40	14.886	2173	2176	2184	rVB7	38491	79008	1.87%	0.169%
41	15.227	2229	2234	2239	rBV	589306	678765	16.03%	1.454%
42	15.316	2246	2249	2254	rVB	39522	48672	1.15%	0.104%
43	15.468	2270	2275	2278	rBV	166871	259389	6.13%	0.556%
44	15.616	2294	2300	2307	rBV	793366	967198	22.84%	2.072%
45	15.786	2325	2329	2336	rVB	77542	94804	2.24%	0.203%
46	15.851	2336	2340	2344	rBV2	47868	75848	1.79%	0.163%
47	15.921	2347	2352	2360	rVB	885428	1101627	26.02%	2.360%
48	16.021	2363	2369	2377	rBV	806811	1090431	25.76%	2.336%
49	16.486	2441	2448	2460	rBV	635860	1050844	24.82%	2.252%
50	17.021	2532	2539	2557	rVB	303269	603547	14.26%	1.293%
51	17.639	2638	2644	2655	rBV2	90922	213340	5.04%	0.457%

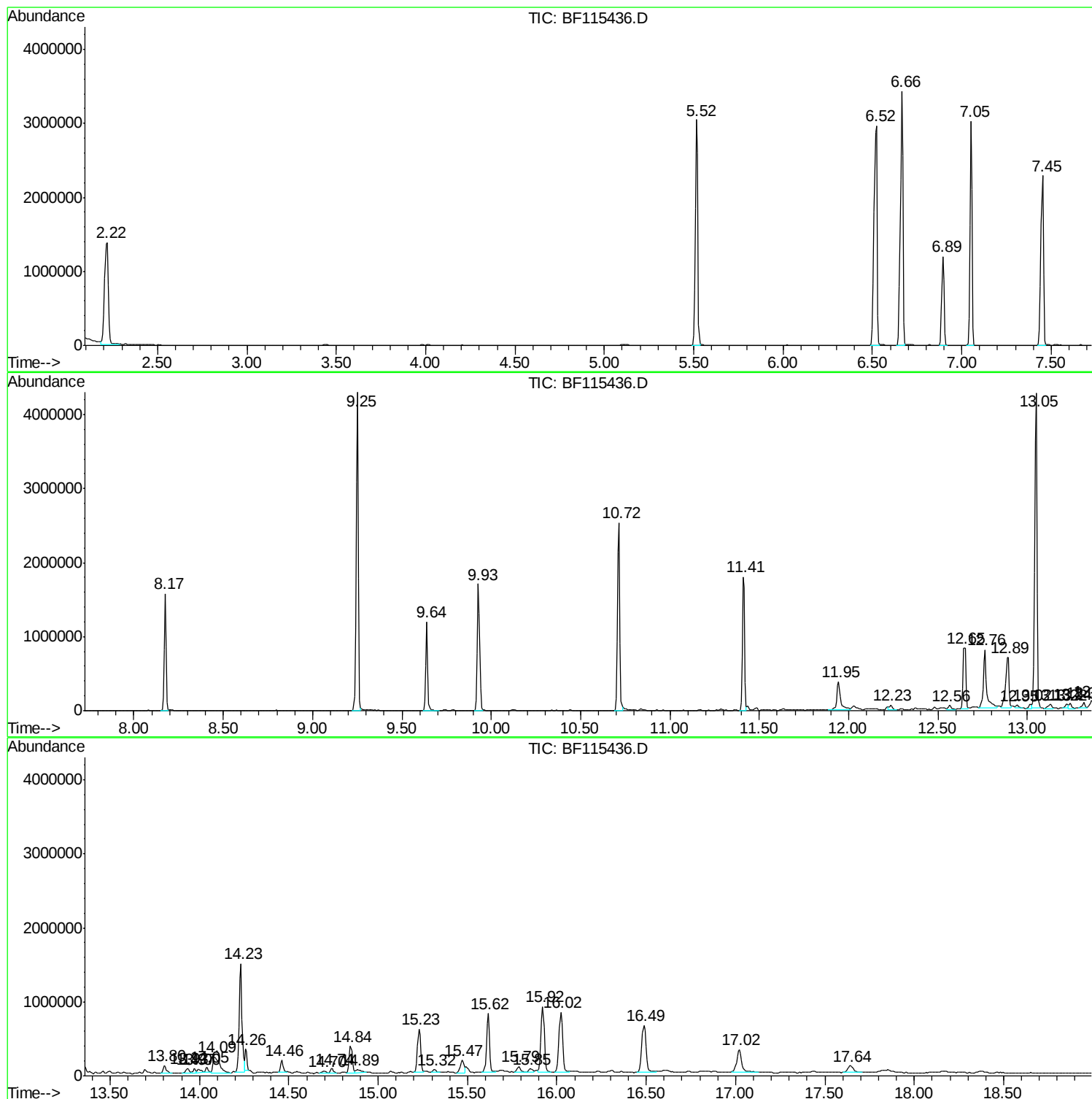
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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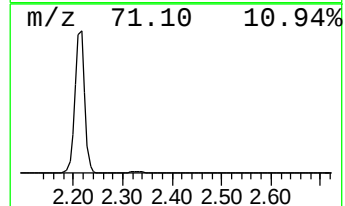
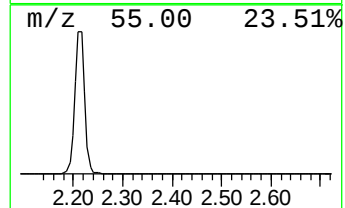
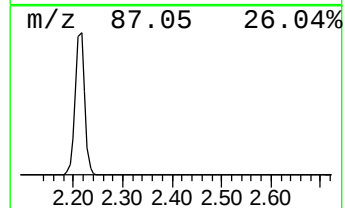
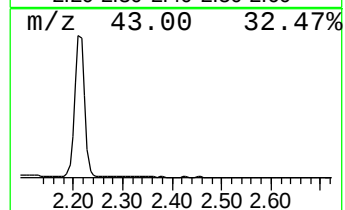
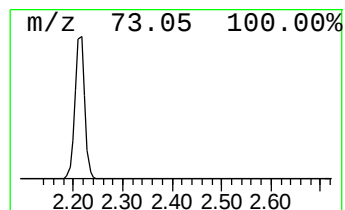
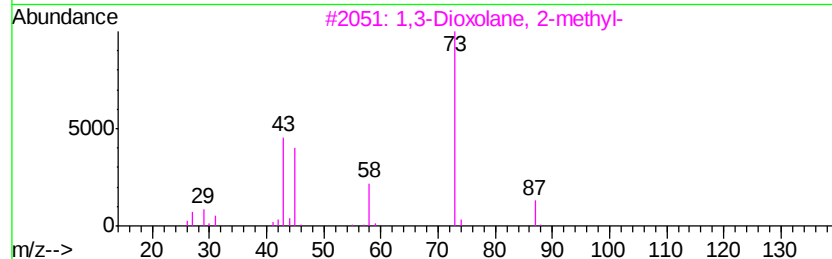
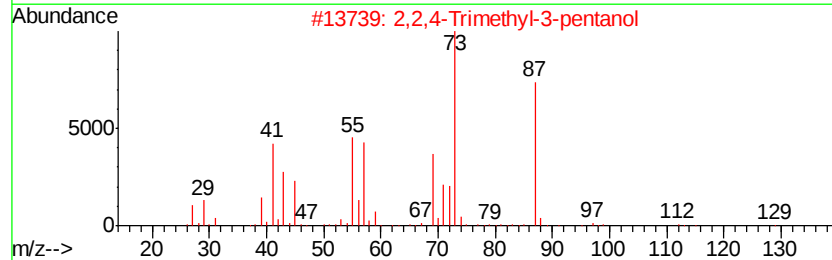
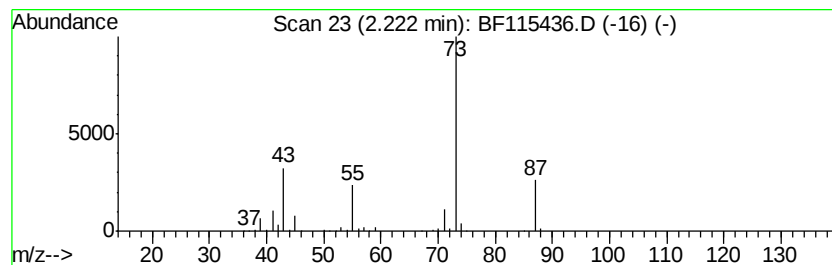
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF070519.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	38.93 ng	1897570	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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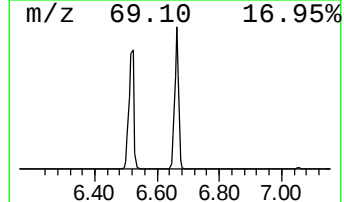
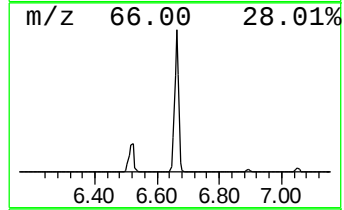
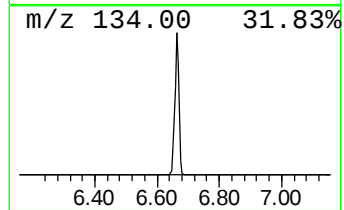
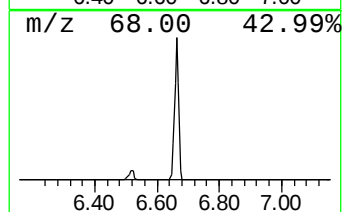
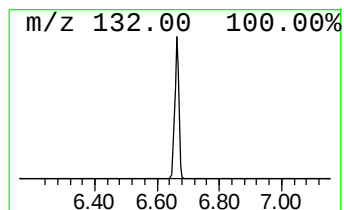
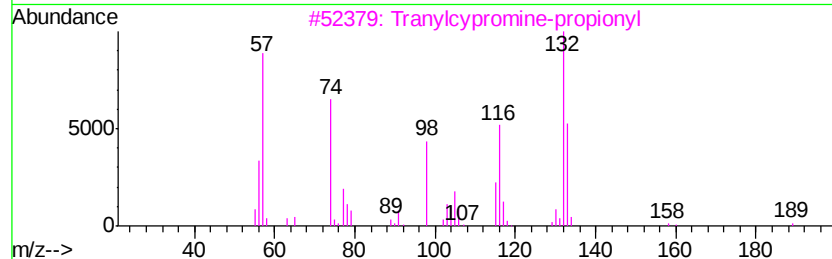
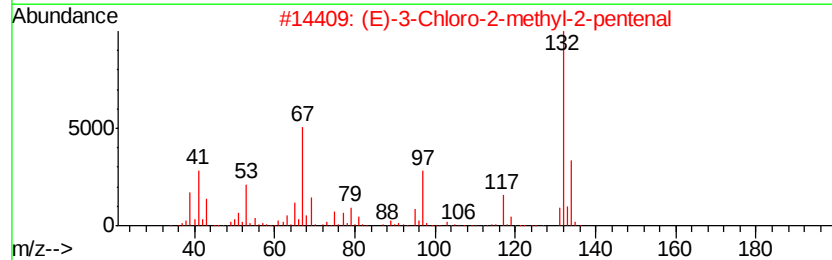
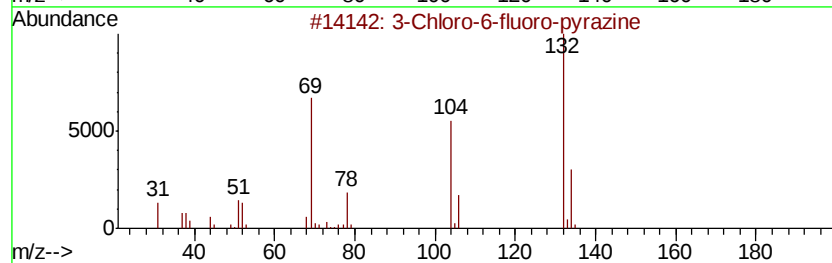
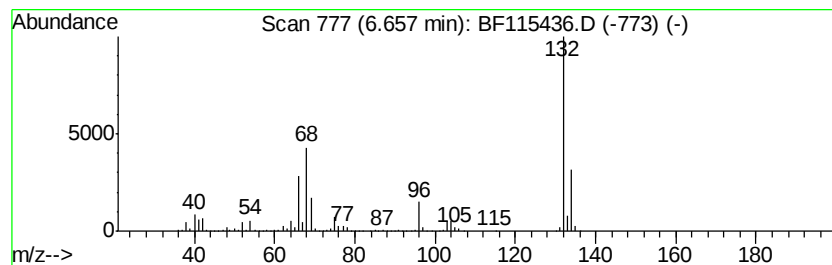
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	68.52 ng	3340330	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Xenon	132	Xe	007440-63-3	9



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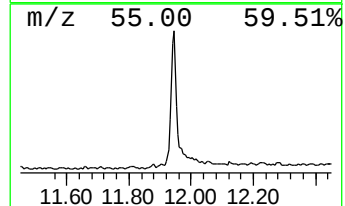
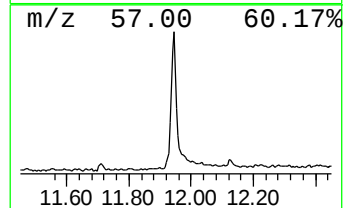
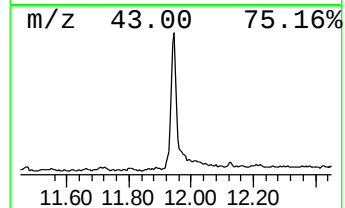
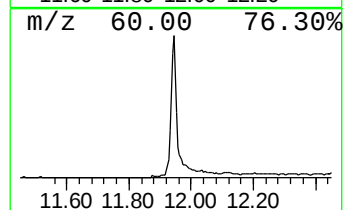
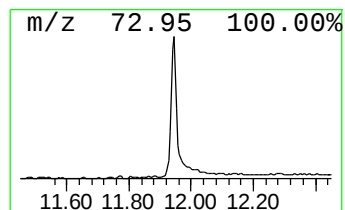
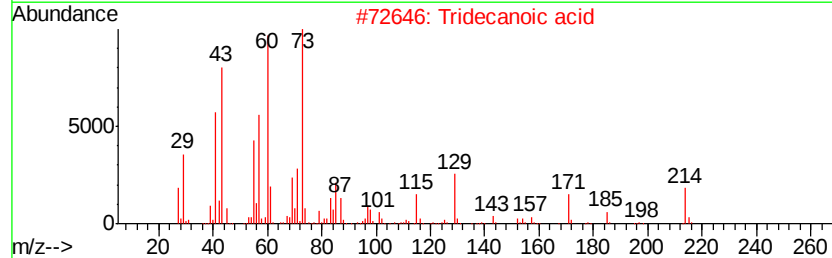
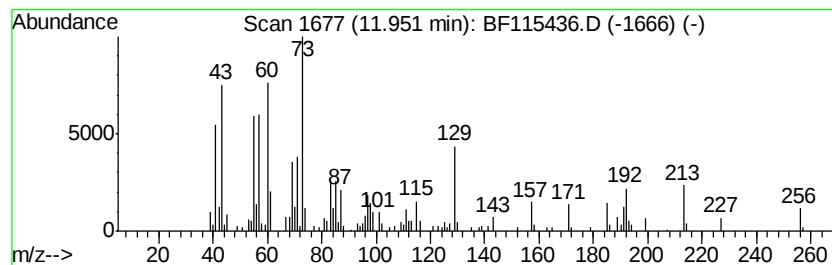
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	6.24 ng	519174	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	15



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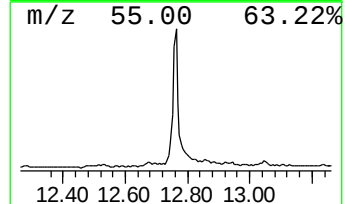
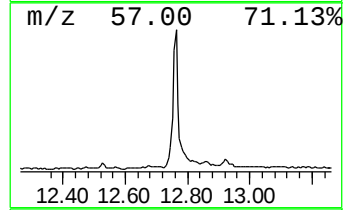
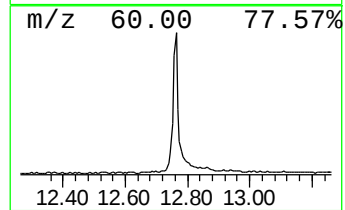
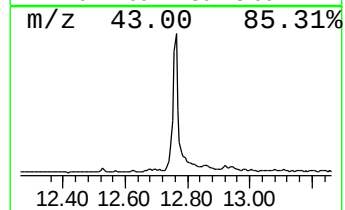
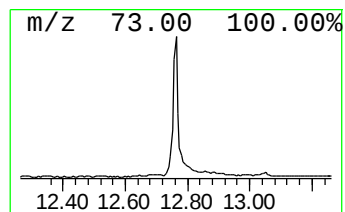
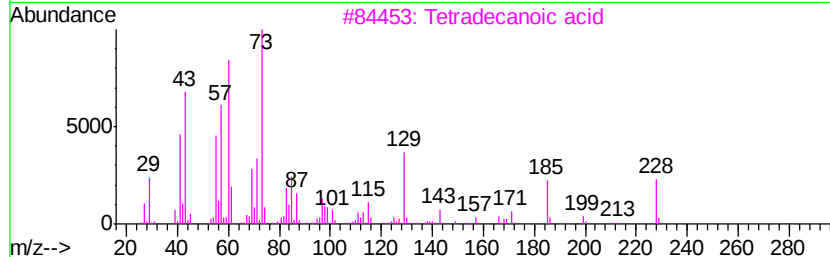
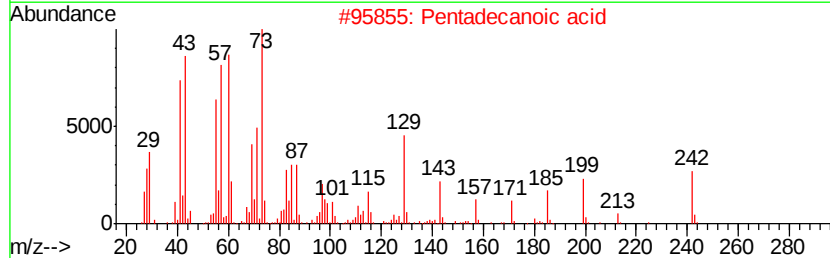
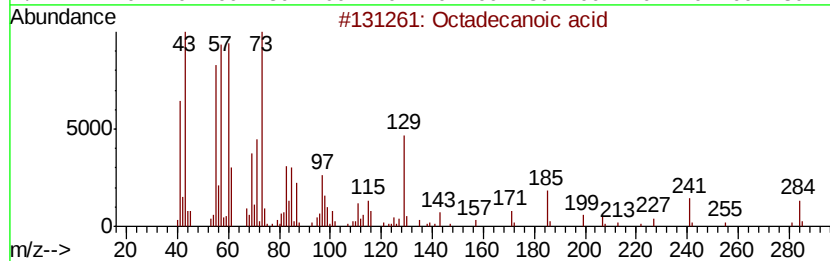
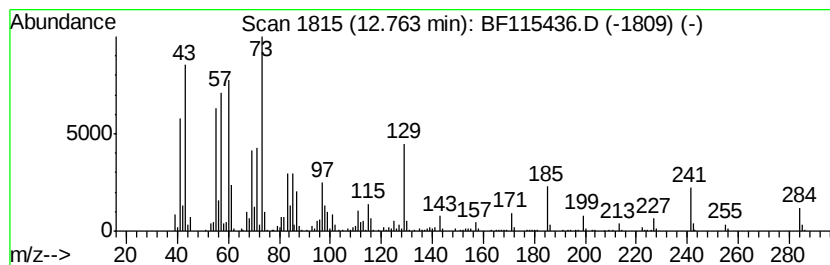
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	12.65 ng	1052280	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	74
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72



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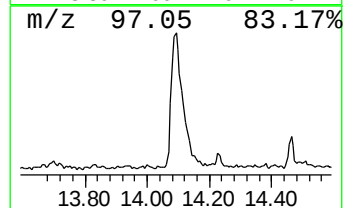
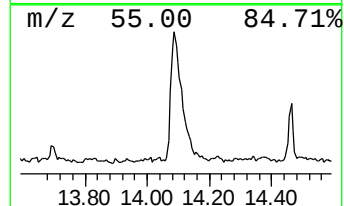
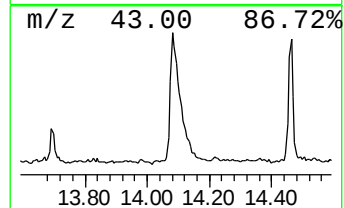
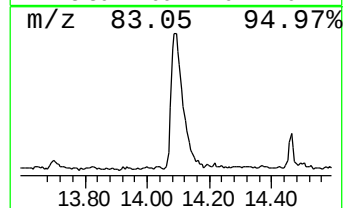
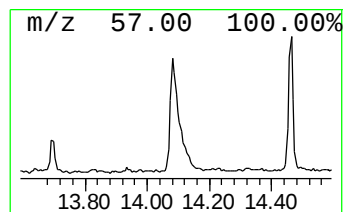
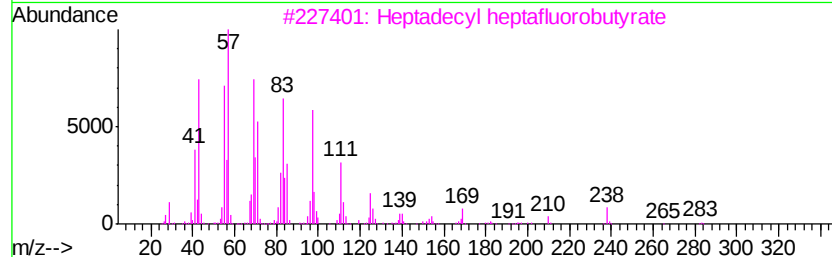
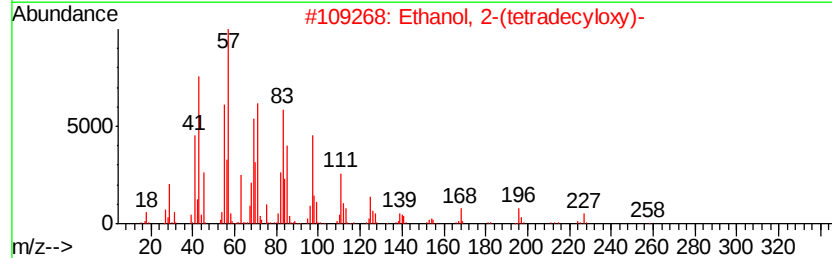
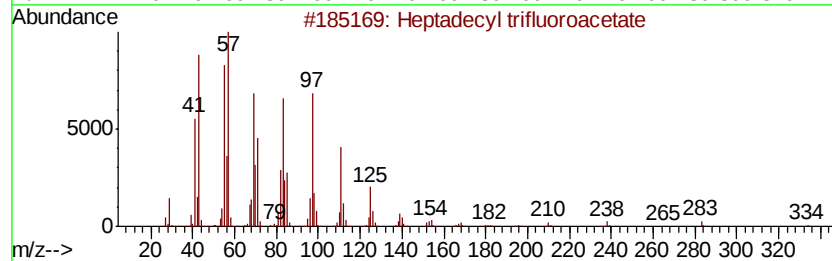
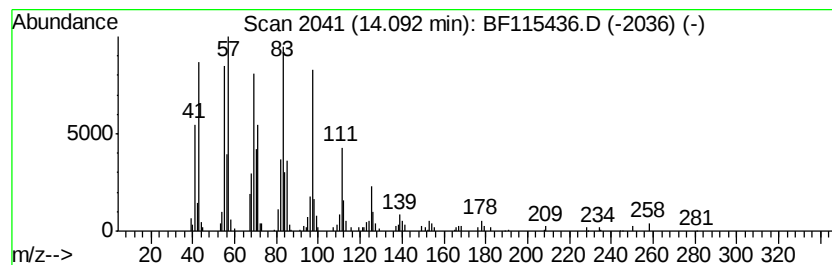
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ClientSampleId :
72-12017-VNJ-206

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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 Heptadecyl trifluoroacetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.09	6.97 ng	570970	Chrysene-d12	14.23		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Heptadecyl heptafluorobutyrte	452	C21H35F7O2	959085-66-6	91
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	81
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
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Acq On : 9 Jul 2019 16:17
Operator : HP/JU
Sample : K3687-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

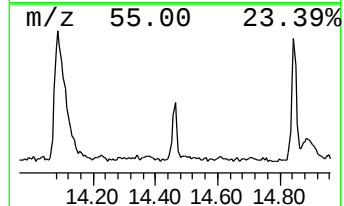
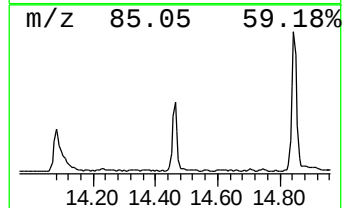
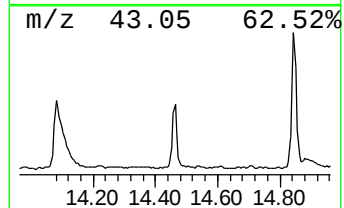
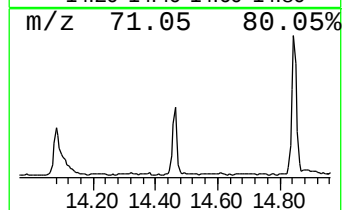
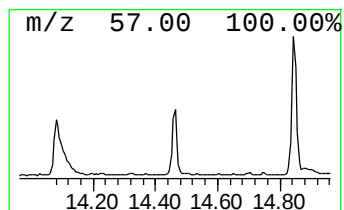
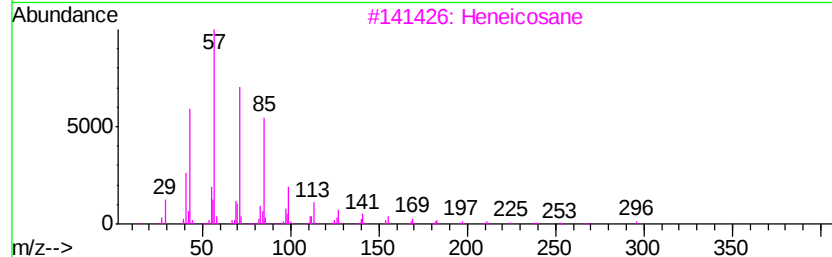
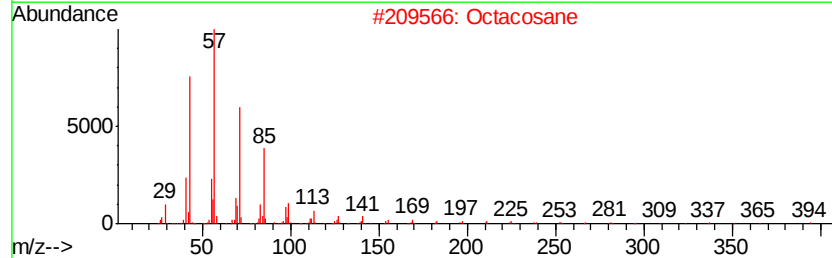
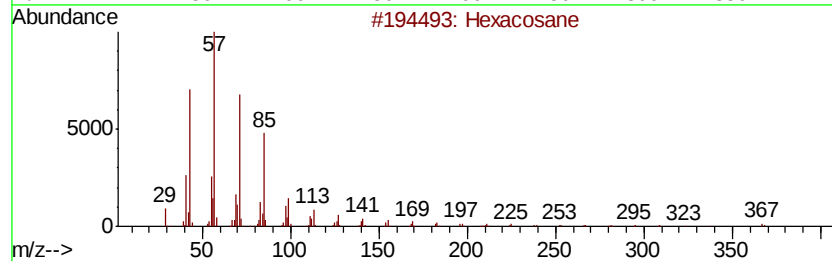
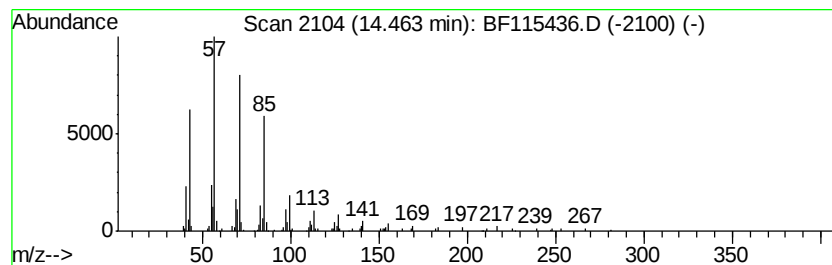
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.13 ng	174190	Chrysene-d12	14.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	91
2	Octacosane	394 C28H58	000630-02-4	91
3	Heneicosane	296 C21H44	000629-94-7	91
4	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
5	Docosane	310 C22H46	000629-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
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Sample : K3687-01
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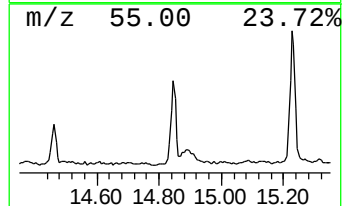
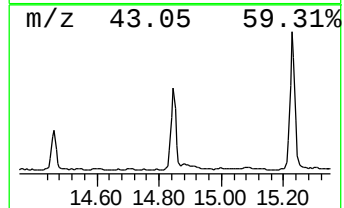
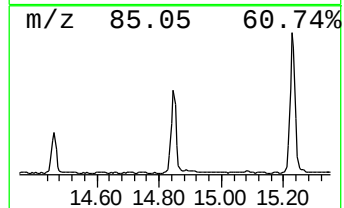
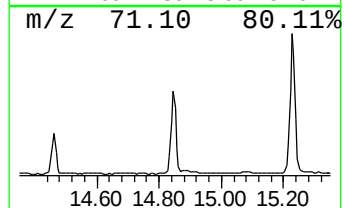
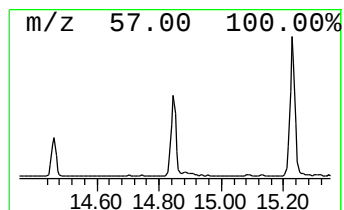
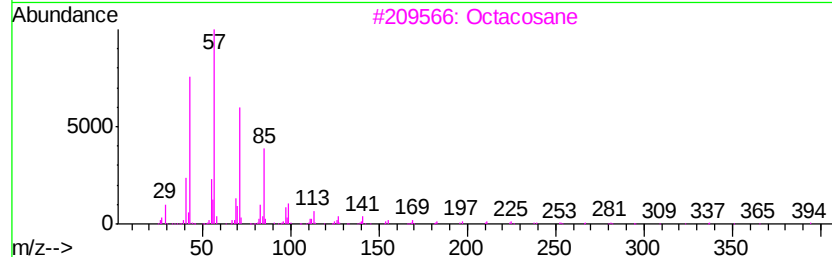
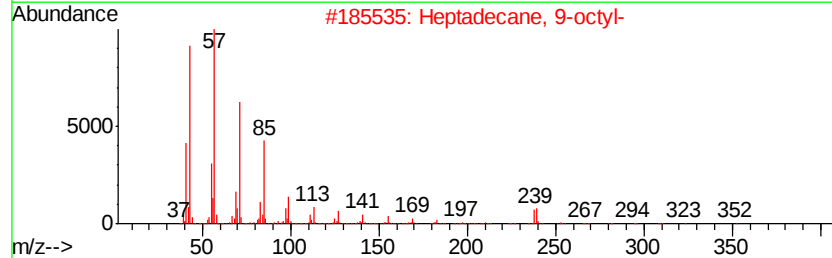
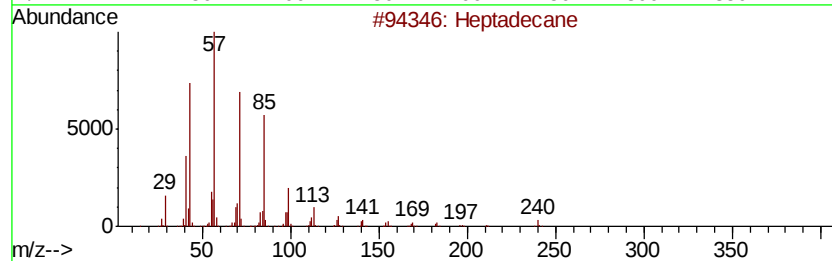
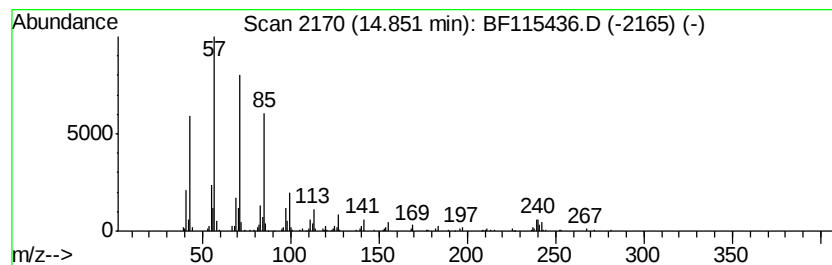
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	4.88 ng	399512	Chrysene-d12	14.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	93
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
3	Octacosane	394 C28H58	000630-02-4	90
4	Hexacosane	366 C26H54	000630-01-3	90
5	Heneicosane	296 C21H44	000629-94-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
Data File : BF115436.D
Acq On : 9 Jul 2019 16:17
Operator : HP/JU
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Instrument :
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ClientSampleId :
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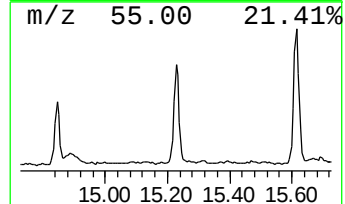
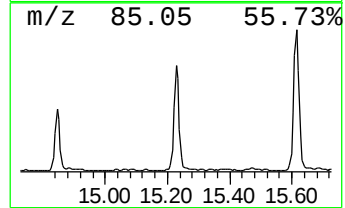
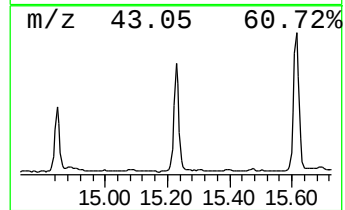
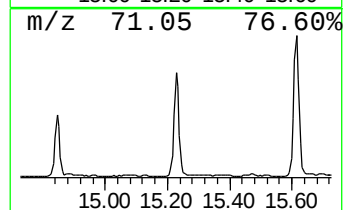
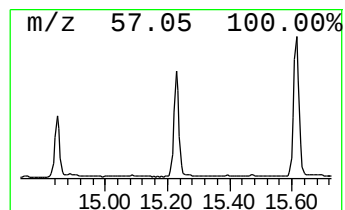
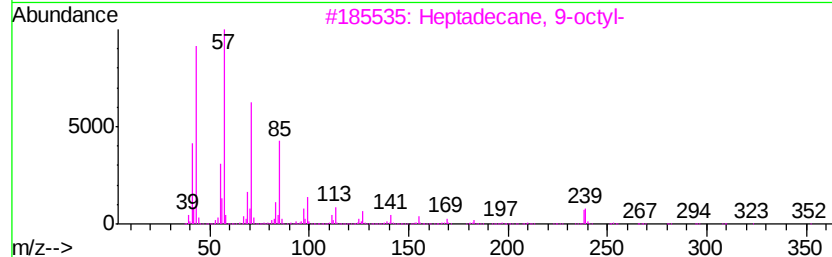
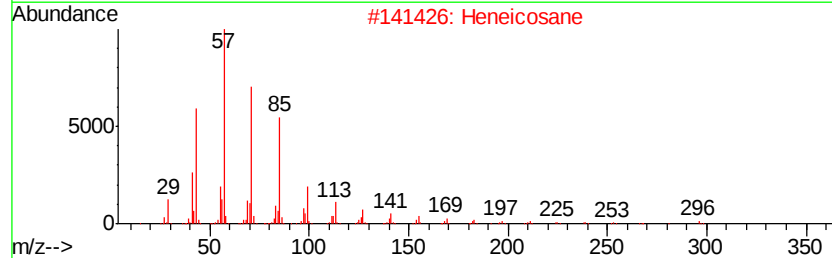
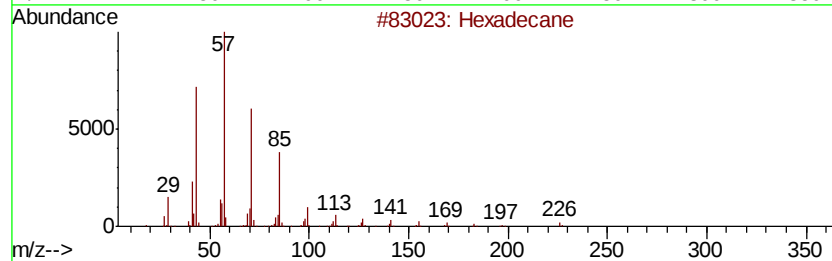
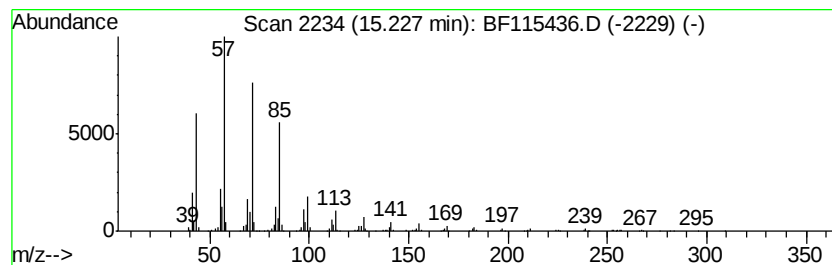
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	12.32 ng	678765	Perylene-d12	15.92

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	93
2	Heneicosane		296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	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\BF070919\
Data File : BF115436.D
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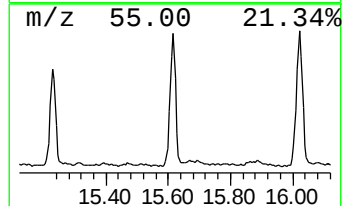
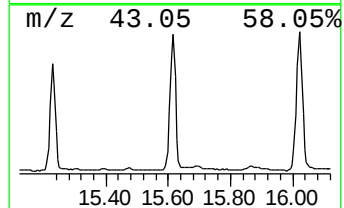
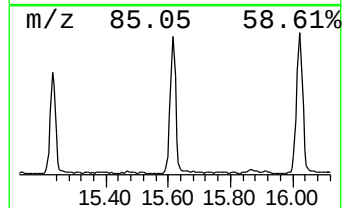
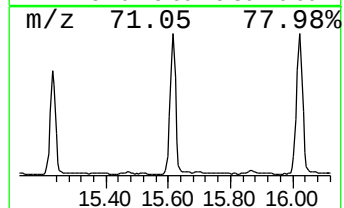
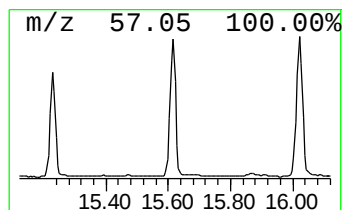
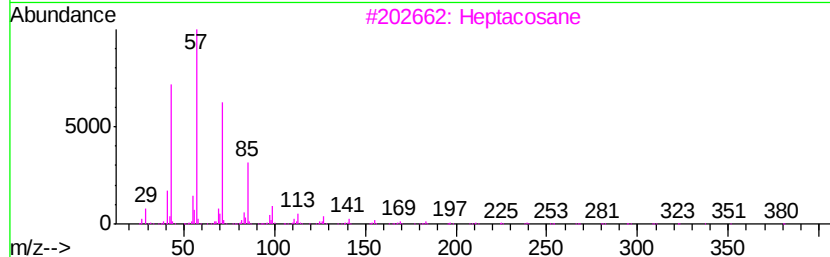
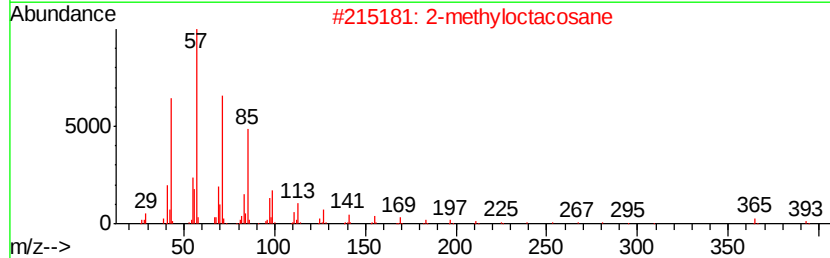
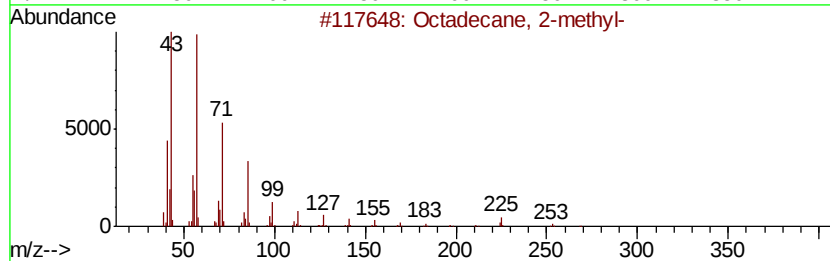
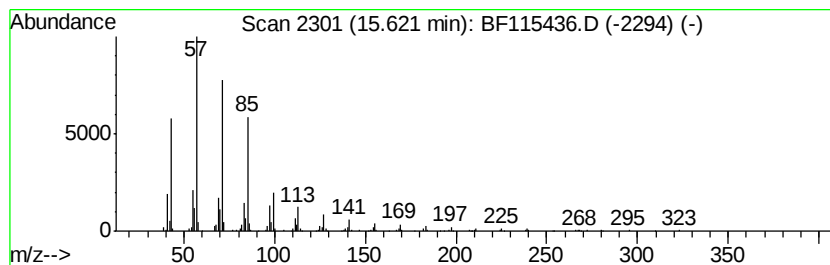
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	17.56 ng	967198	Perylene-d12	15.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
Data File : BF115436.D
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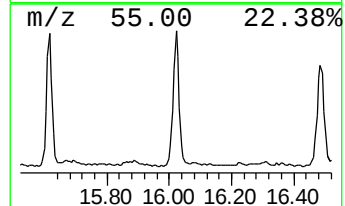
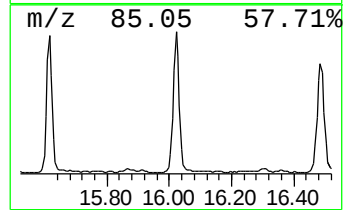
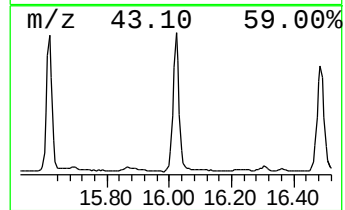
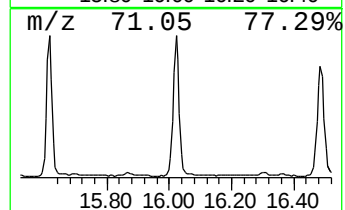
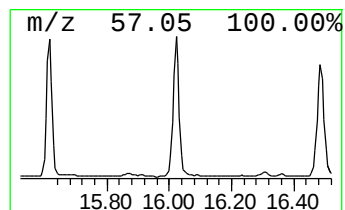
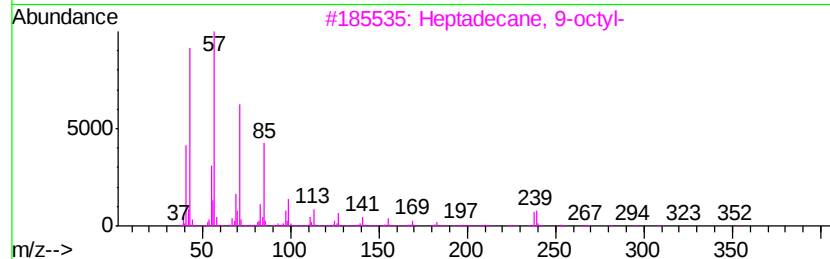
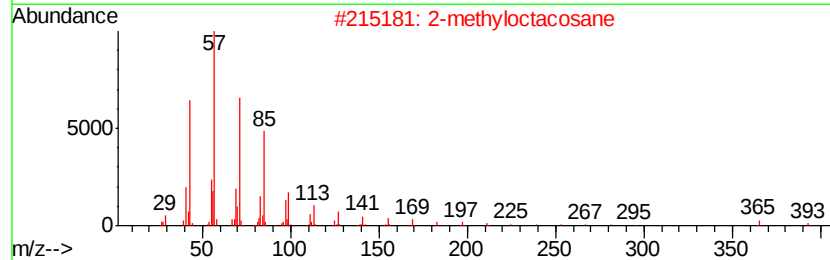
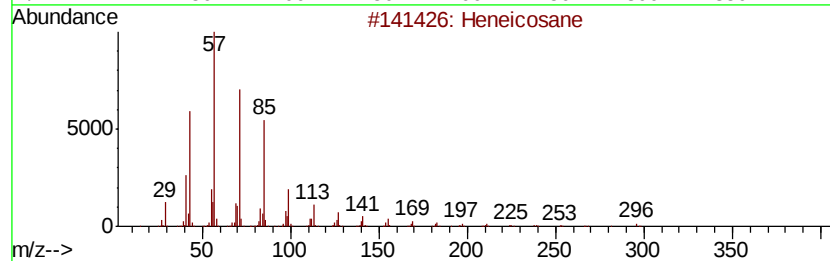
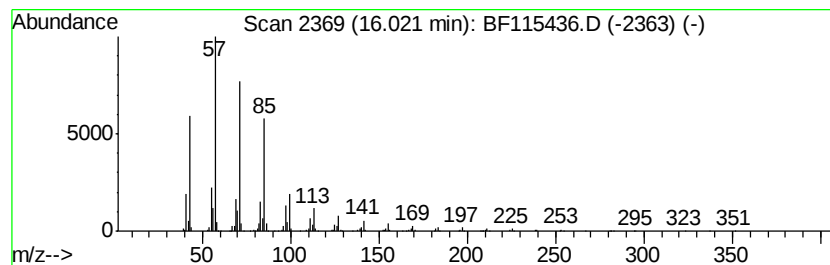
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	19.80 ng	1090430	Perylene-d12	15.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Hexacosane	366	C26H54	000630-01-3	90



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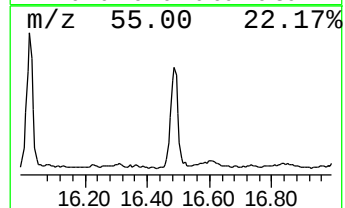
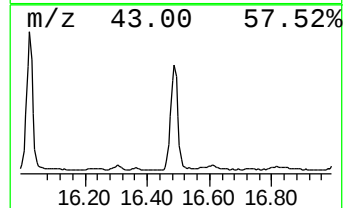
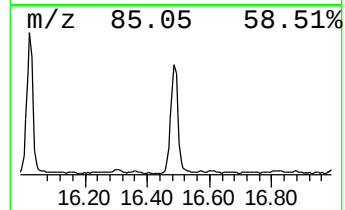
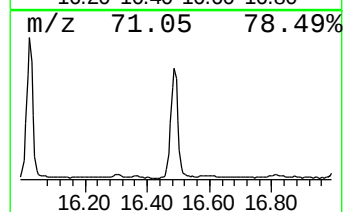
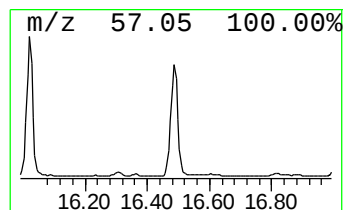
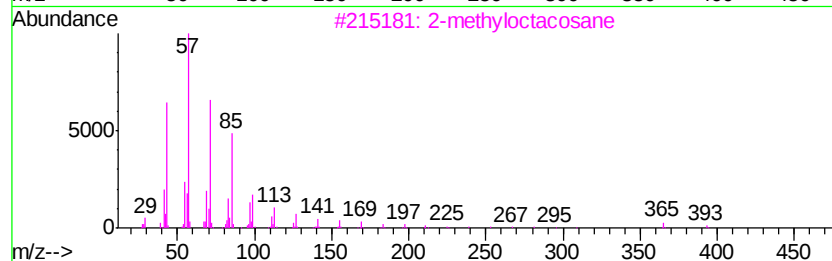
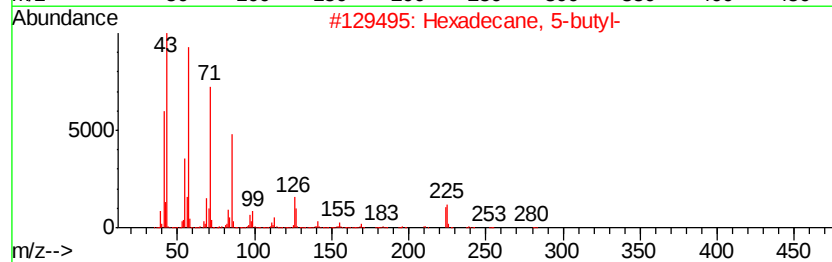
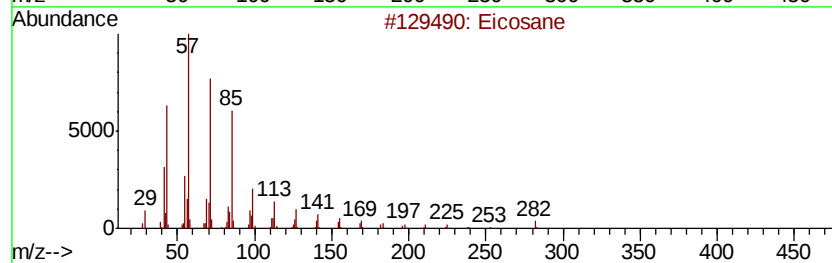
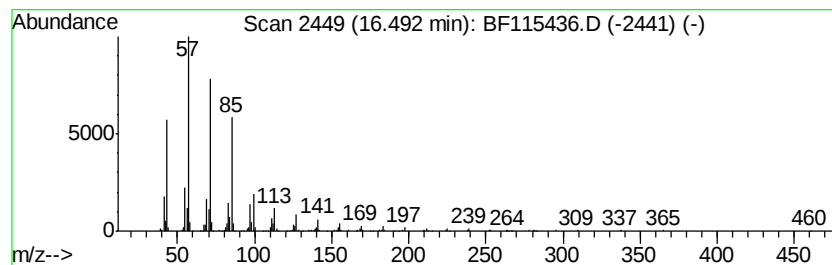
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	19.08 ng	1050840	Perylene-d12	15.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Hexadecane, 5-butyl-	282 C20H42	006912-07-8	93
3	2-methyloctacosane	408 C29H60	1000376-72-8	91
4	Heneicosane	296 C21H44	000629-94-7	91
5	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
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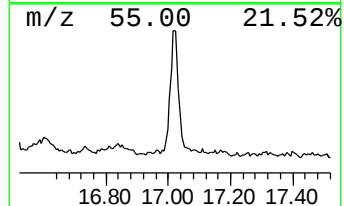
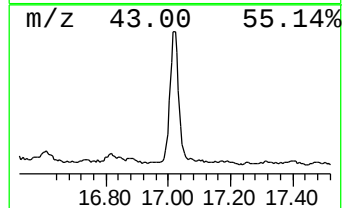
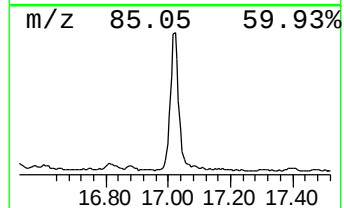
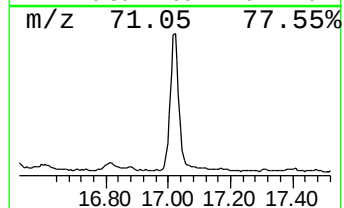
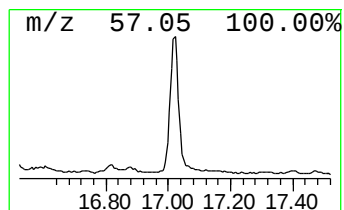
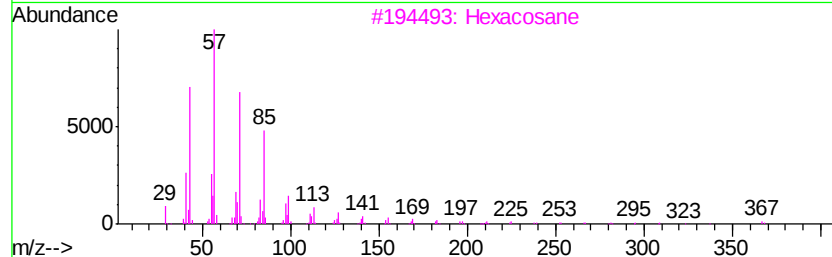
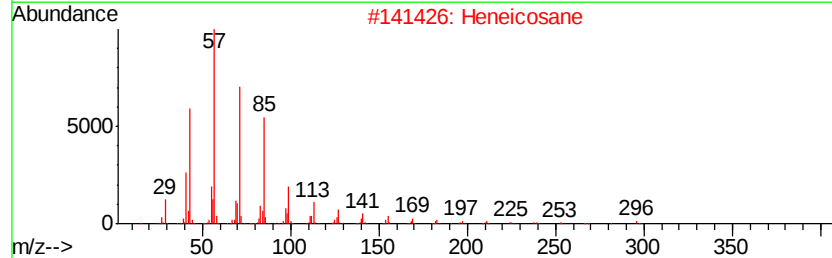
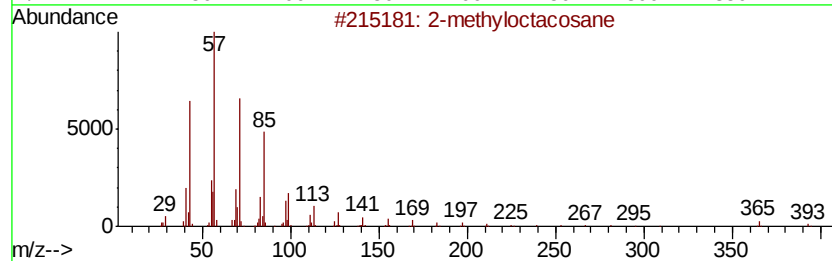
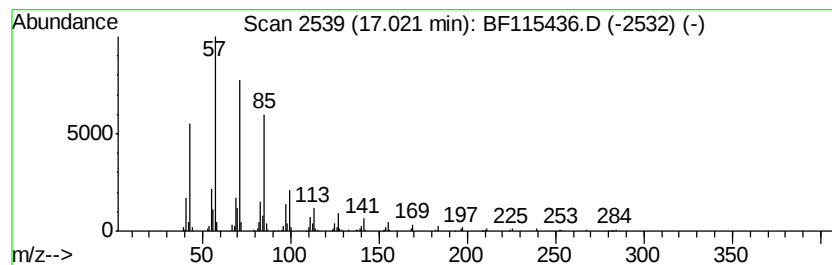
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-methyloctacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.02	10.96 ng	603547	Perylene-d12	15.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF070919\
Data File : BF115436.D
Acq On : 9 Jul 2019 16:17
Operator : HP/JU
Sample : K3687-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12017-VNJ-206

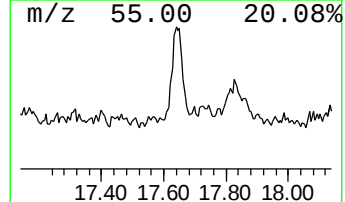
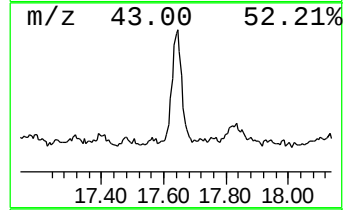
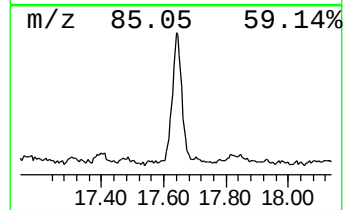
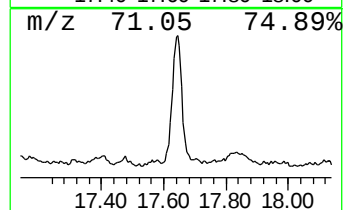
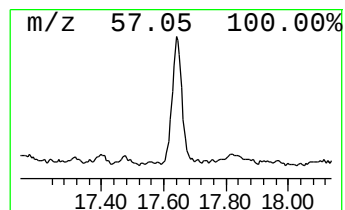
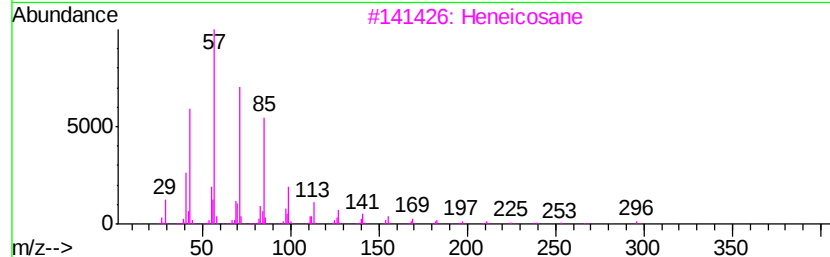
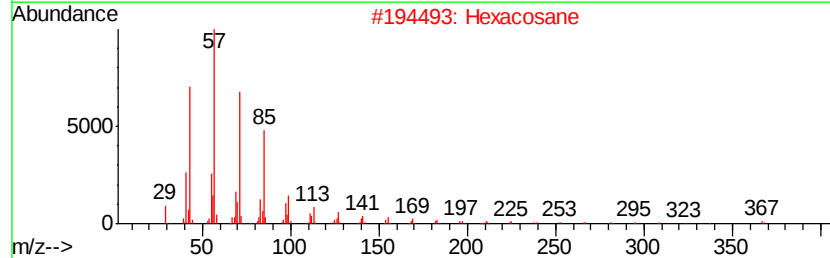
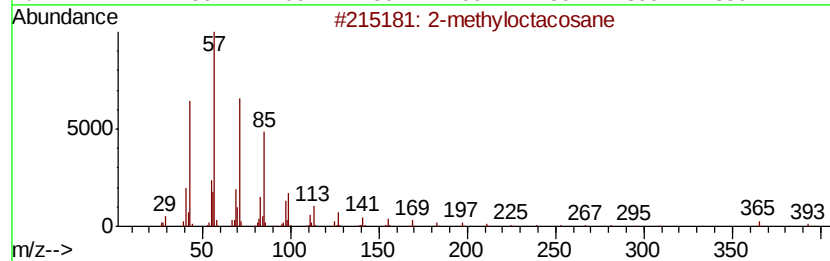
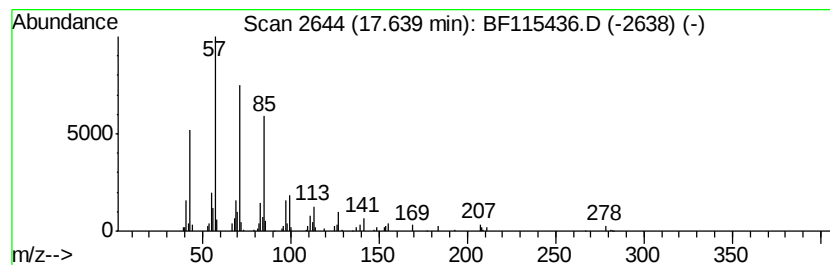
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF070519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heptadecane, 9-hexyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	3.87 ng	213340	Perylene-d12	15.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF070919\
Data File : BF115436.D
Acq On : 9 Jul 2019 16:17
Operator : HP/JU
Sample : K3687-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-12017-VNJ-206

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF070519.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
Butane, 2-methoxy...	2.22	38.9	ng	1897570	1	6.89	974987	20.0
unknown6.66	6.66	68.5	ng	3340330	1	6.89	974987	20.0
n-Hexadecanoic acid	11.95	6.2	ng	519174	4	11.41	1663670	20.0
Octadecanoic acid	12.76	12.7	ng	1052280	4	11.41	1663670	20.0
Heptadecyl triflu...	14.09	7.0	ng	570970	5	14.23	1637760	20.0
Hexacosane	14.46	2.1	ng	174190	5	14.23	1637760	20.0
Heptadecane	14.85	4.9	ng	399512	5	14.23	1637760	20.0
Hexadecane	15.23	12.3	ng	678765	6	15.92	1101630	20.0
Octadecane, 2-met...	15.62	17.6	ng	967198	6	15.92	1101630	20.0
Heneicosane	16.02	19.8	ng	1090430	6	15.92	1101630	20.0
Eicosane	16.49	19.1	ng	1050840	6	15.92	1101630	20.0
2-methyloctacosane	17.02	11.0	ng	603547	6	15.92	1101630	20.0
Heptadecane, 9-he...	17.64	3.9	ng	213340	6	15.92	1101630	20.0