

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083019\
 Data File : BF116673.D
 Acq On : 31 Aug 2019 1:58
 Operator : HP/JU
 Sample : K4517-12
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T4-S-D1-D4

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	5.457	568	573	577	rBV	2153720	2072636	87.68%	7.634%
2	6.469	740	745	750	rBV	2216898	2363877	100.00%	8.707%
3	6.616	765	770	773	rBV	2498560	2258646	95.55%	8.319%
4	6.845	805	809	812	rBV	836605	648336	27.43%	2.388%
5	7.004	832	836	839	rBV	2109341	1681182	71.12%	6.192%
6	7.404	899	904	907	rBV	1671378	1451619	61.41%	5.347%
7	8.128	1023	1027	1030	rBV	1042349	859149	36.34%	3.165%
8	9.198	1205	1209	1213	rBV	2529747	2329783	98.56%	8.581%
9	9.586	1272	1275	1279	rBV	211678	184042	7.79%	0.678%
10	9.880	1321	1325	1328	rBV	1141772	982349	41.56%	3.618%
11	10.663	1454	1458	1461	rBV	1581945	1384720	58.58%	5.100%
12	10.763	1471	1475	1477	rBV	35494	34098	1.44%	0.126%
13	11.357	1572	1576	1579	rBV	1080457	1002223	42.40%	3.692%
14	11.380	1579	1580	1583	rVV	223007	139905	5.92%	0.515%
15	11.427	1583	1588	1591	rVB3	37315	49930	2.11%	0.184%
16	11.586	1610	1615	1618	rBV2	21046	26056	1.10%	0.096%
17	11.857	1658	1661	1663	rBV	30248	28250	1.20%	0.104%
18	11.886	1663	1666	1673	rVV	317982	292876	12.39%	1.079%
19	11.974	1678	1681	1682	rBV2	37834	36391	1.54%	0.134%
20	12.174	1712	1715	1718	rVB	66066	61254	2.59%	0.226%
21	12.486	1765	1768	1775	rVB	45017	52054	2.20%	0.192%
22	12.568	1778	1782	1785	rVV	657739	548195	23.19%	2.019%
23	12.668	1796	1799	1802	rBV2	108092	105521	4.46%	0.389%
24	12.798	1814	1821	1824	rBV	495036	551846	23.34%	2.033%
25	12.845	1826	1829	1835	rVB2	30840	33410	1.41%	0.123%
26	12.915	1838	1841	1842	rBV2	36733	33709	1.43%	0.124%
27	12.939	1842	1845	1849	rVV	2132357	2064700	87.34%	7.605%
28	13.015	1853	1858	1861	rBV2	36529	55768	2.36%	0.205%
29	13.098	1869	1872	1874	rBV2	29771	32182	1.36%	0.119%
30	13.121	1874	1876	1879	rVB	52029	42478	1.80%	0.156%
31	13.186	1884	1887	1890	rVB2	28369	30453	1.29%	0.112%
32	13.227	1890	1894	1896	rBV2	56951	63834	2.70%	0.235%
33	13.315	1907	1909	1912	rBV	26380	25158	1.06%	0.093%
34	13.351	1912	1915	1919	rBV3	24475	28145	1.19%	0.104%

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ClientSampleId :
T4-S-D1-D4

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	13.421	1924	1927	1931	rVB6	22808	27896	1.18%	0.103%
36	13.621	1958	1961	1965	rVB	87328	98227	4.16%	0.362%
37	13.739	1976	1981	1983	rBV2	58240	80300	3.40%	0.296%
38	13.768	1983	1986	1988	rVV	54808	49752	2.10%	0.183%
39	13.792	1988	1990	1994	rVV2	42860	53708	2.27%	0.198%
40	13.833	1994	1997	2006	rVB2	433257	464869	19.67%	1.712%
41	13.992	2018	2024	2026	rBV2	870230	1056444	44.69%	3.891%
42	14.015	2026	2028	2034	rVB	337405	289868	12.26%	1.068%
43	14.162	2049	2053	2057	rVB3	64130	77986	3.30%	0.287%
44	14.204	2057	2060	2064	rBV2	35519	39267	1.66%	0.145%
45	14.374	2085	2089	2092	rVB	40959	44820	1.90%	0.165%
46	14.410	2092	2095	2099	rVB	69865	60814	2.57%	0.224%
47	14.468	2099	2105	2108	rBV2	110692	128504	5.44%	0.473%
48	14.574	2118	2123	2126	rVB4	21071	33320	1.41%	0.123%
49	14.668	2137	2139	2143	rBV3	22849	27408	1.16%	0.101%
50	14.768	2151	2156	2160	rBV	104477	115338	4.88%	0.425%
51	14.845	2165	2169	2177	rBV5	51875	87542	3.70%	0.322%
52	15.021	2194	2199	2202	rBV2	290855	481907	20.39%	1.775%
53	15.104	2208	2213	2221	rBV3	103441	180806	7.65%	0.666%
54	15.227	2229	2234	2240	rVB7	31902	60534	2.56%	0.223%
55	15.315	2245	2249	2255	rVB	176421	219725	9.30%	0.809%
56	15.374	2255	2259	2265	rBV	209294	256640	10.86%	0.945%
57	15.445	2265	2271	2274	rBV	613720	764423	32.34%	2.816%
58	15.480	2274	2277	2284	rVB3	126074	190241	8.05%	0.701%
59	15.915	2346	2351	2355	rBV	78437	116100	4.91%	0.428%
60	15.962	2355	2359	2363	rBV6	34562	58711	2.48%	0.216%
61	16.409	2431	2435	2439	rBV2	37137	67208	2.84%	0.248%
62	16.874	2509	2514	2524	rVB2	121885	233314	9.87%	0.859%
63	17.109	2549	2554	2559	rBV3	20722	34340	1.45%	0.126%
64	17.309	2582	2588	2598	rVB	100372	194304	8.22%	0.716%

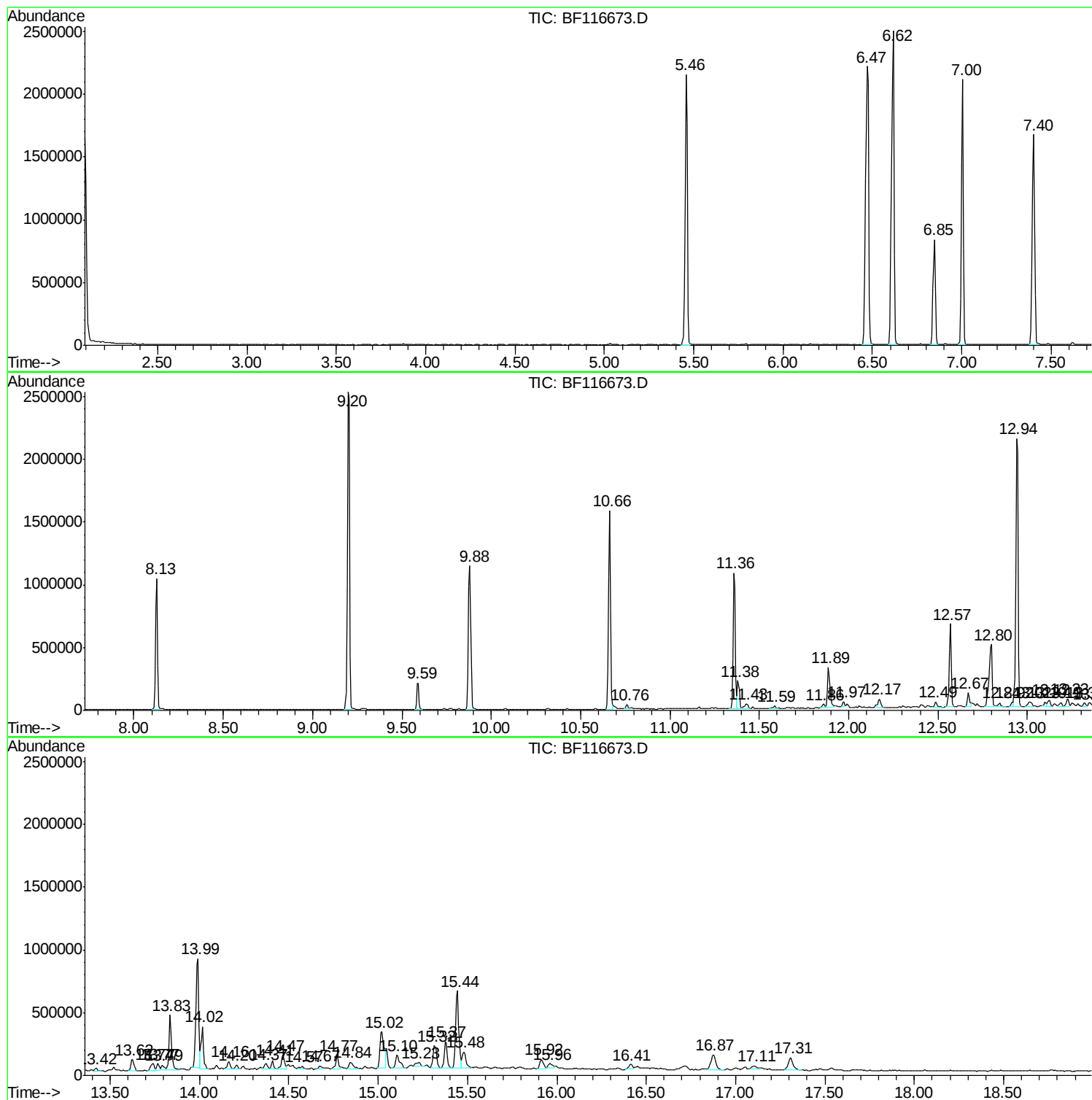
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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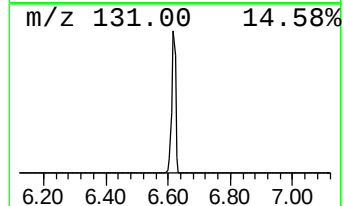
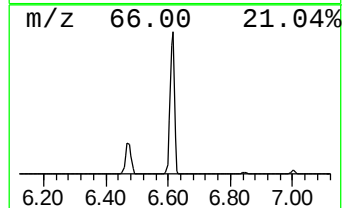
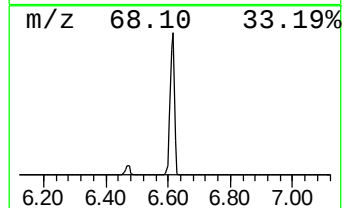
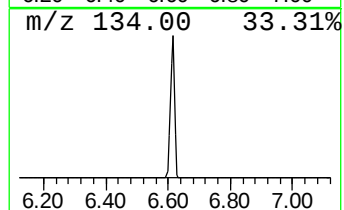
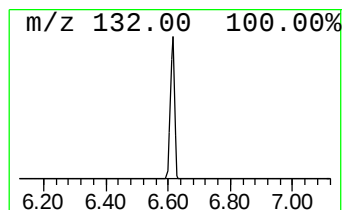
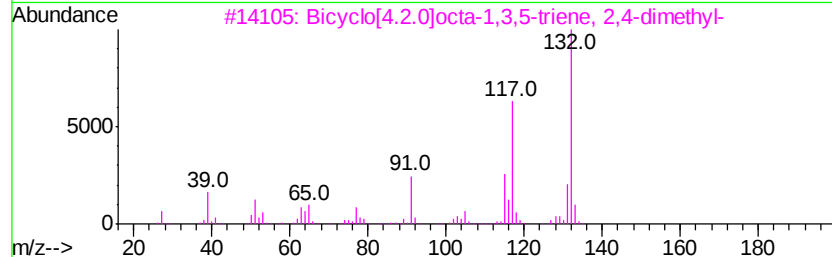
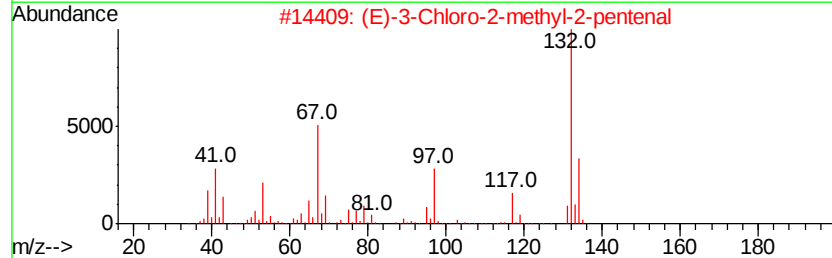
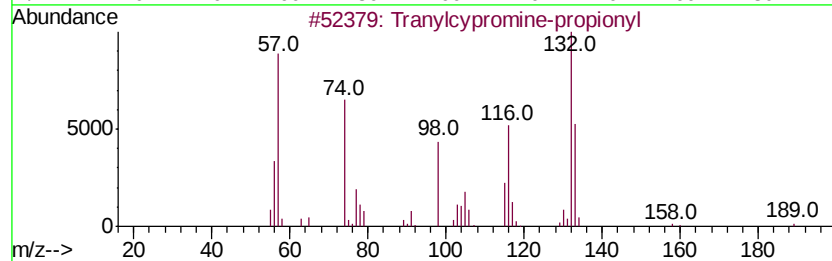
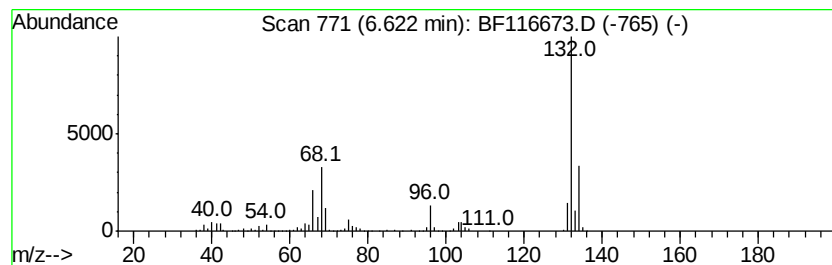
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	69.68 ng	2258650	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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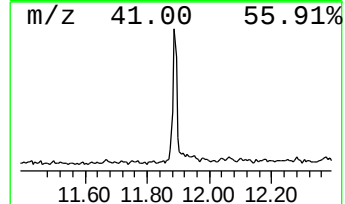
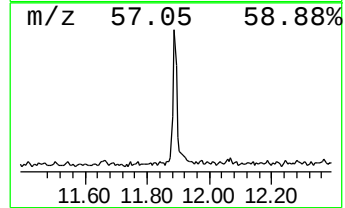
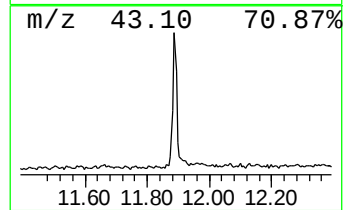
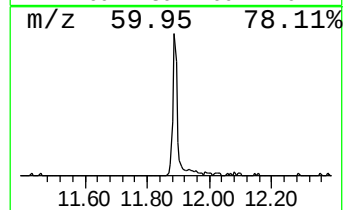
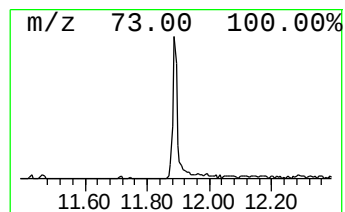
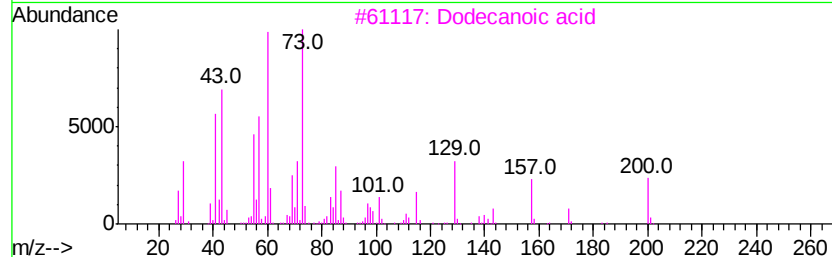
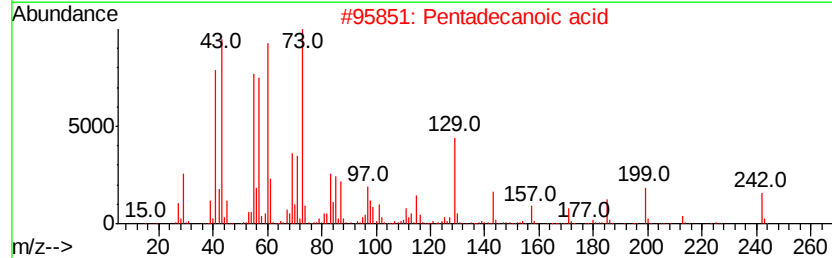
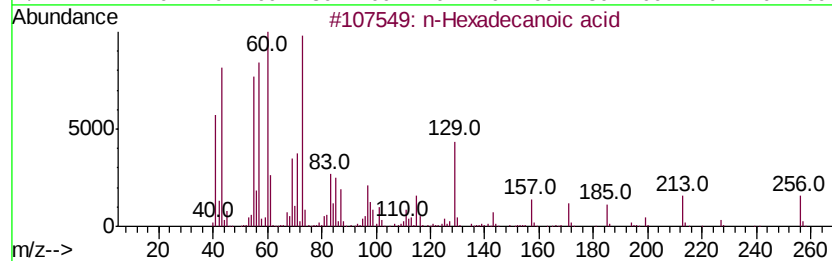
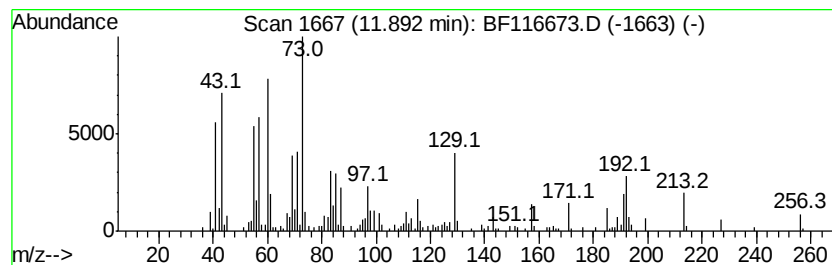
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	5.84 ng	292876	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
3		Dodecanoic acid	200	C12H24O2	000143-07-7	52
4		Tridecane	184	C13H28	000629-50-5	11
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	11



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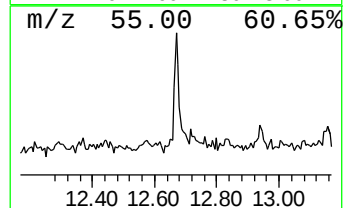
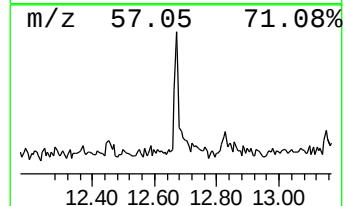
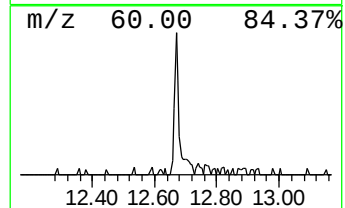
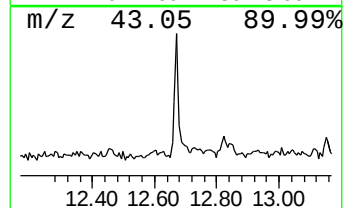
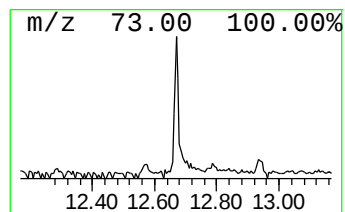
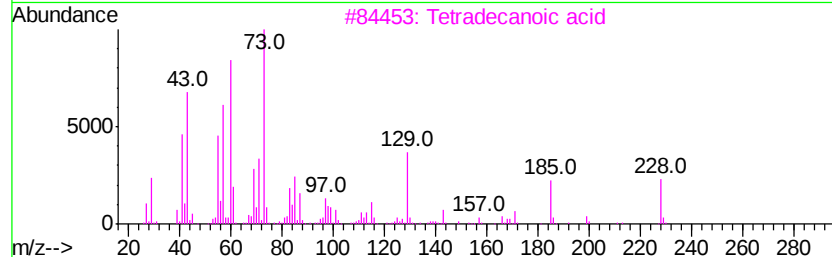
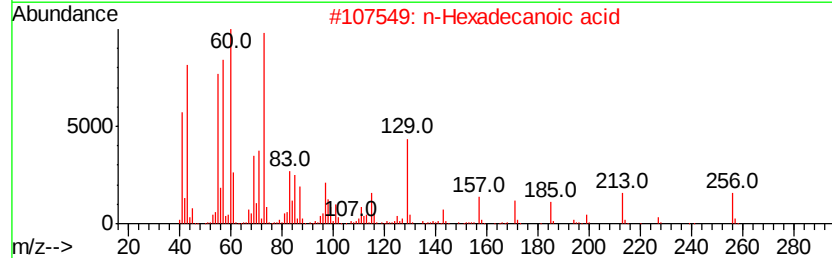
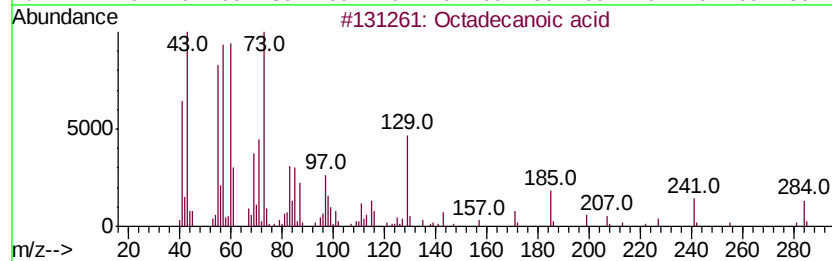
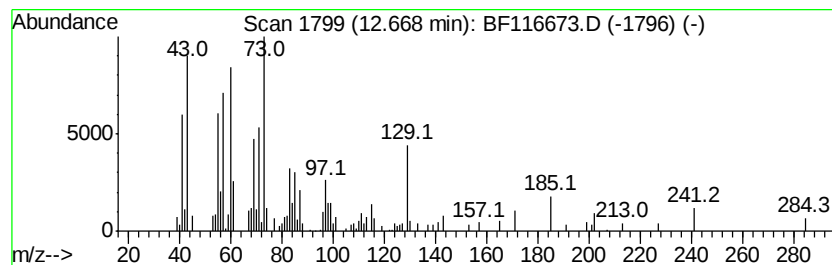
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	2.11 ng	105521	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	72
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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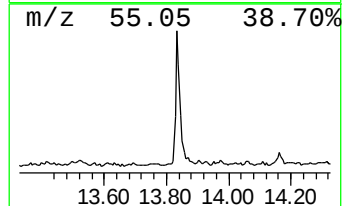
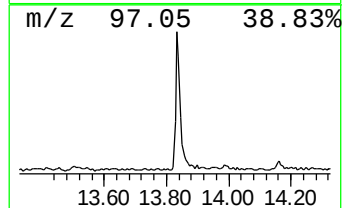
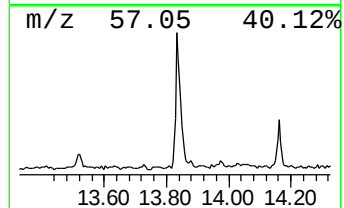
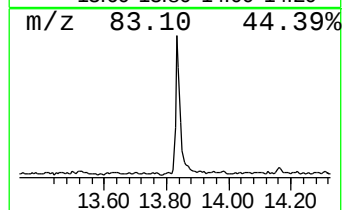
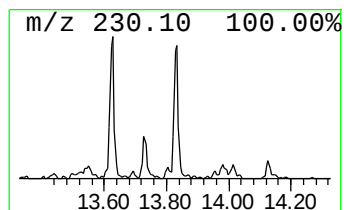
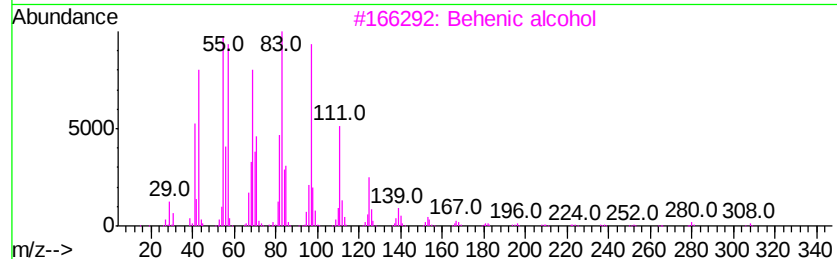
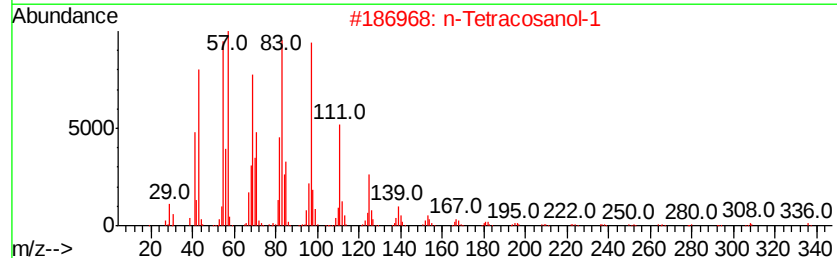
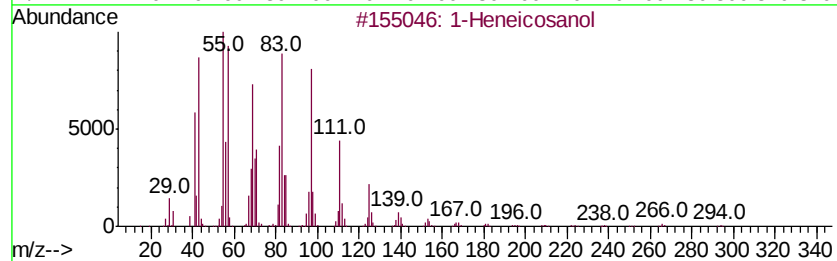
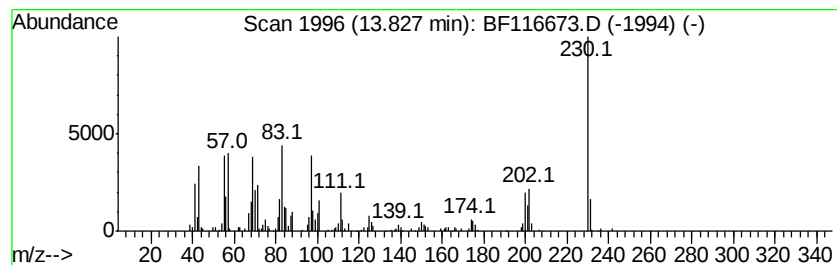
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.83	8.80 ng	464869	Chrysene-d12	13.99	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	89



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ClientSampleId :
T4-S-D1-D4

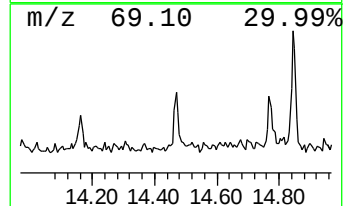
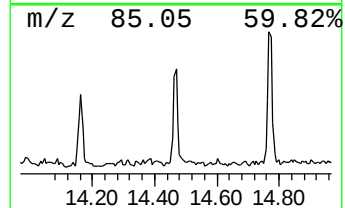
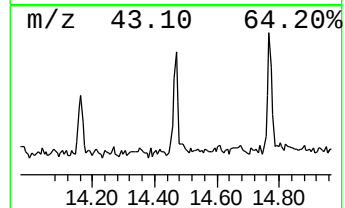
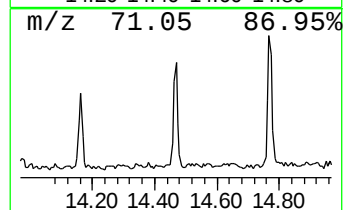
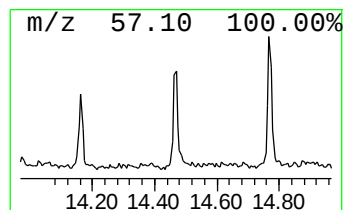
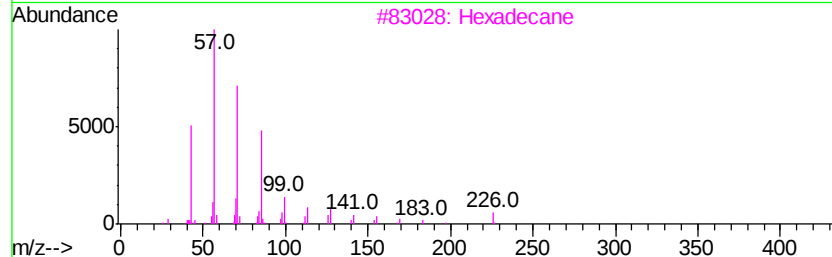
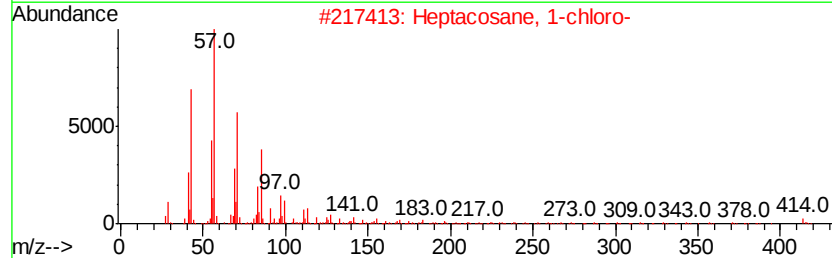
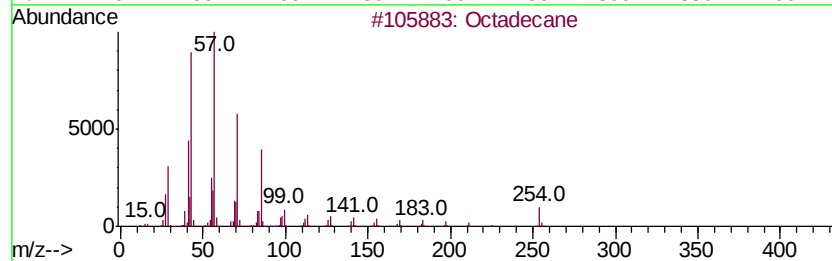
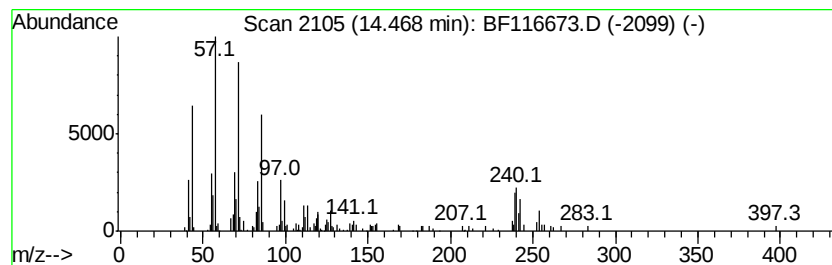
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.43 ng	128504	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	78
2	Heptacosane, 1-chloro-		414	C27H55Cl	062016-79-9	58
3	Hexadecane		226	C16H34	000544-76-3	55
4	Hexacosane		366	C26H54	000630-01-3	53
5	Tritetracontane		605	C43H88	007098-21-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083019\
Data File : BF116673.D
Acq On : 31 Aug 2019 1:58
Operator : HP/JU
Sample : K4517-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T4-S-D1-D4

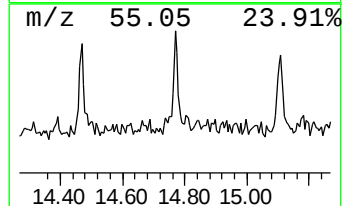
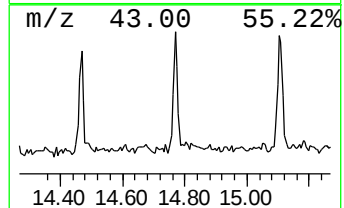
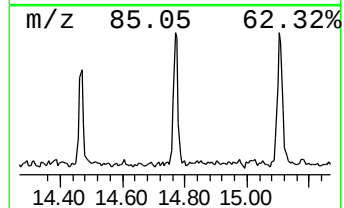
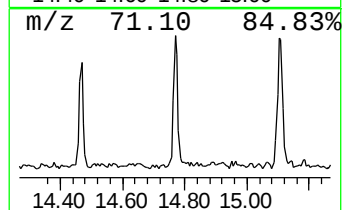
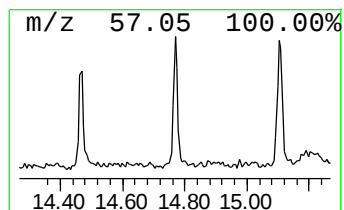
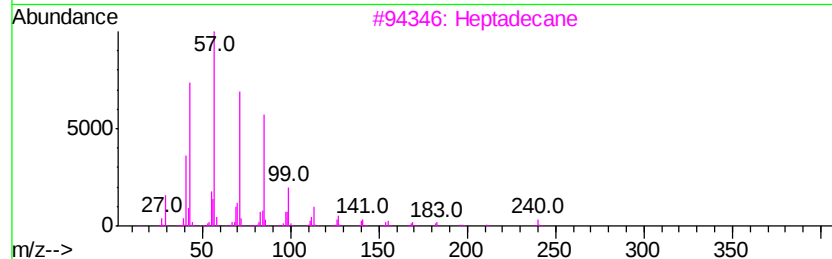
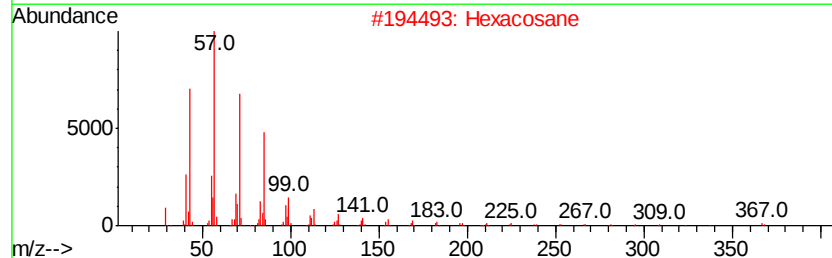
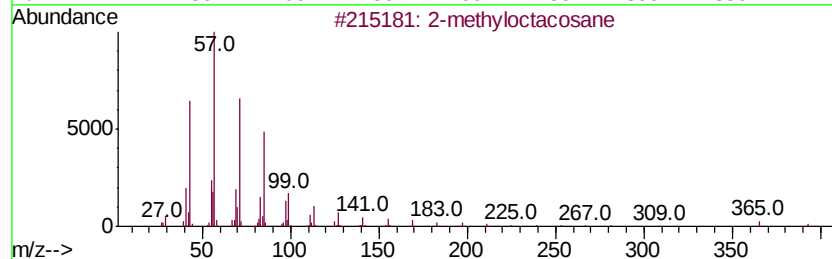
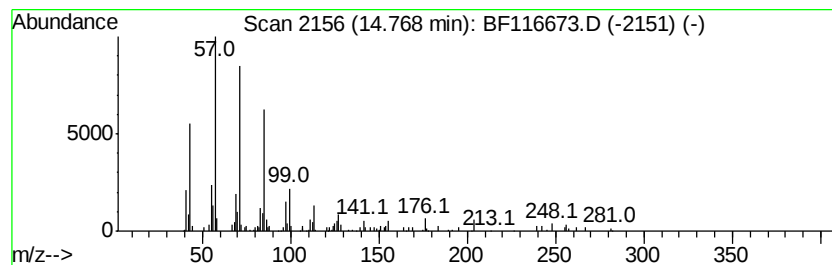
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	3.02 ng	115338	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Hexacosane	366	C26H54	000630-01-3	87
3		Heptadecane	240	C17H36	000629-78-7	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5		Tetratetracontane	619	C44H90	007098-22-8	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083019\
Data File : BF116673.D
Acq On : 31 Aug 2019 1:58
Operator : HP/JU
Sample : K4517-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

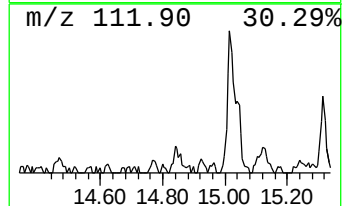
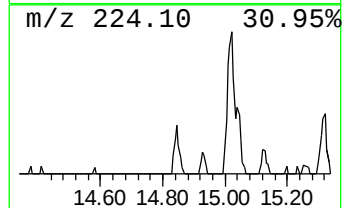
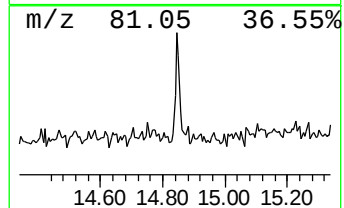
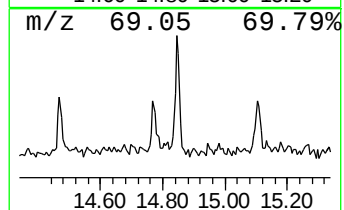
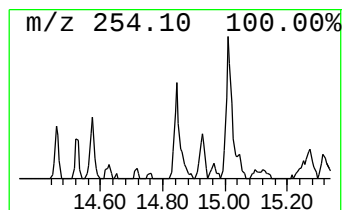
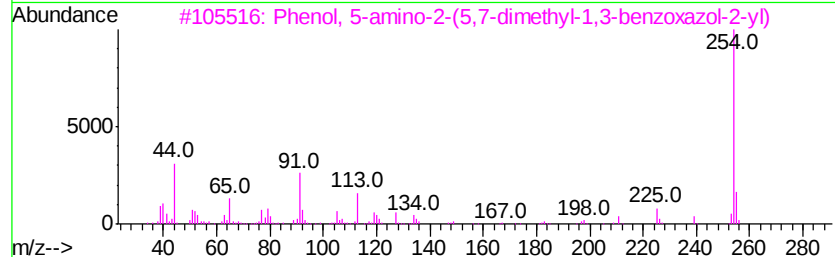
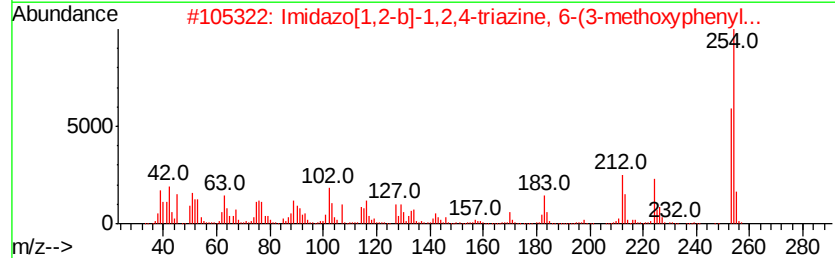
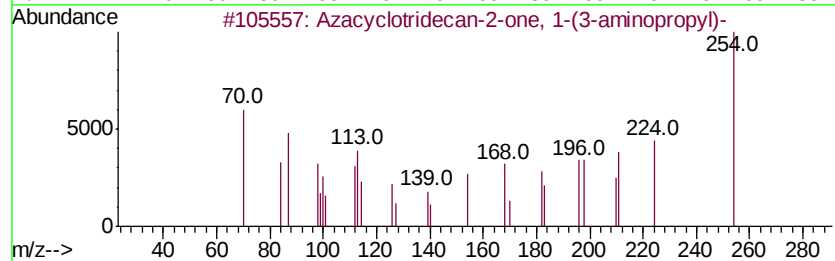
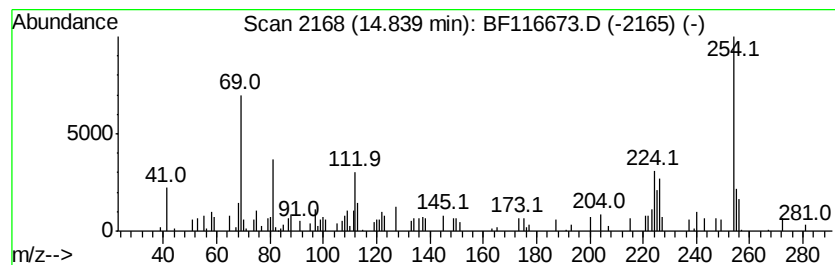
Instrument :
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ClientSampleId :
T4-S-D1-D4

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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 Azacyclotridecan-2-one, 1-(... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.84	2.29 ng	87542	Perylene-d12	15.44		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Azacyclotridecan-2-one, 1-(3-ami...	254	C15H30N2O	064414-61-5	64
2		Imidazo[1,2-b]-1,2,4-triazine, 6...	254	C14H14N4O	1000277-24-4	35
3		Phenol, 5-amino-2-(5,7-dimethyl-...	254	C15H14N2O2	1000338-06-4	30
4		2,2'-Binaphthalene	254	C20H14	000612-78-2	30
5		1,2'-Binaphthalene	254	C20H14	004325-74-0	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083019\
Data File : BF116673.D
Acq On : 31 Aug 2019 1:58
Operator : HP/JU
Sample : K4517-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T4-S-D1-D4

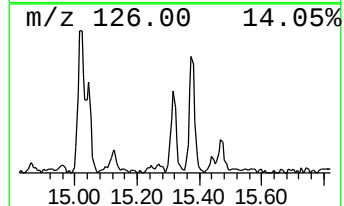
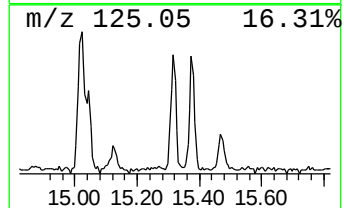
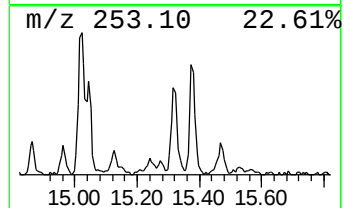
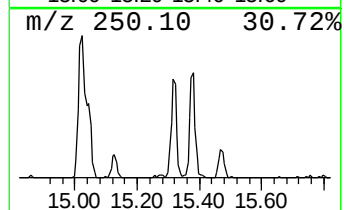
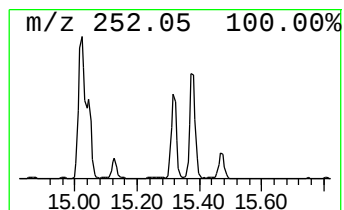
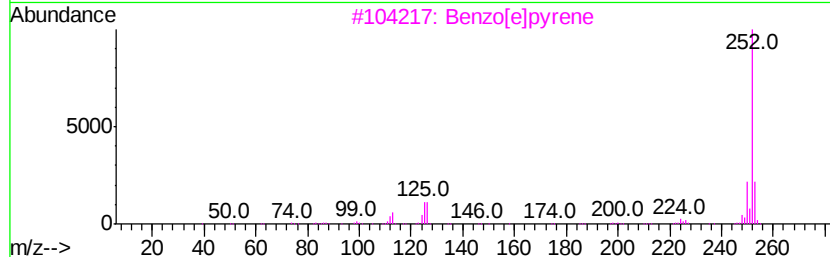
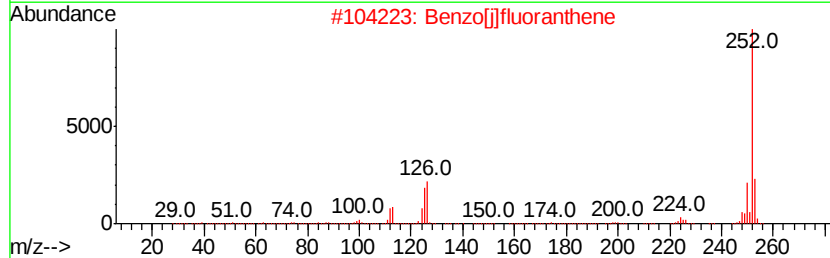
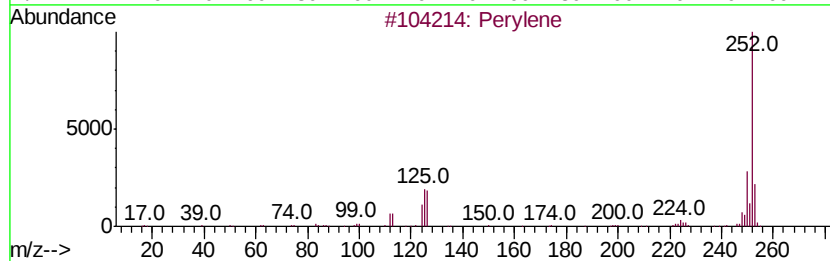
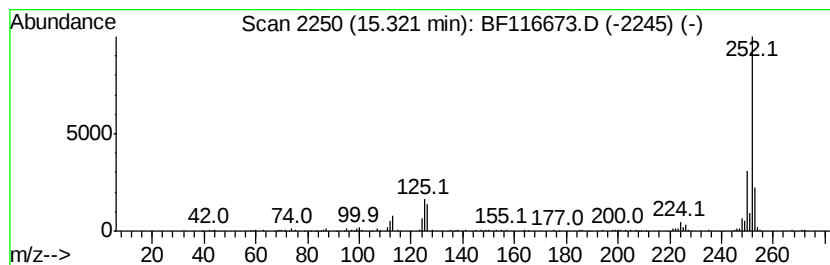
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Perylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.32	5.75 ng	219725	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Perylene	252	C20H12	000198-55-0	98
2		Benzo[il]fluoranthene	252	C20H12	000205-82-3	98
3		Benzo[el]pyrene	252	C20H12	000192-97-2	98
4		Benzo[el]acephenanthrylene	252	C20H12	000205-99-2	97
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083019\
Data File : BF116673.D
Acq On : 31 Aug 2019 1:58
Operator : HP/JU
Sample : K4517-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T4-S-D1-D4

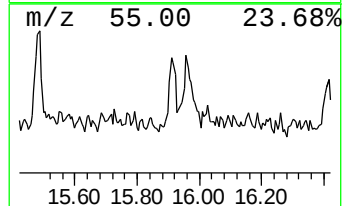
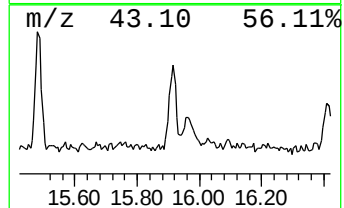
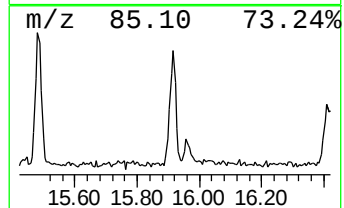
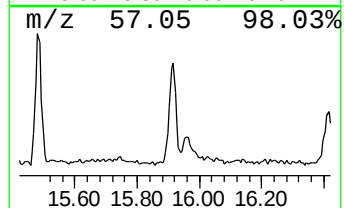
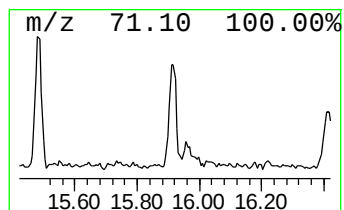
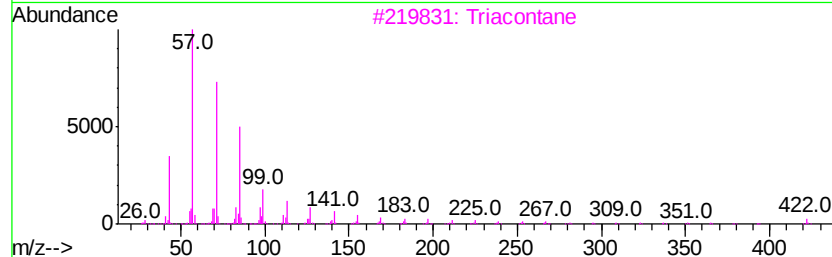
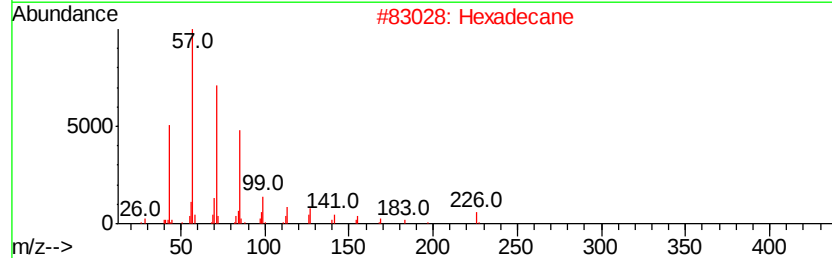
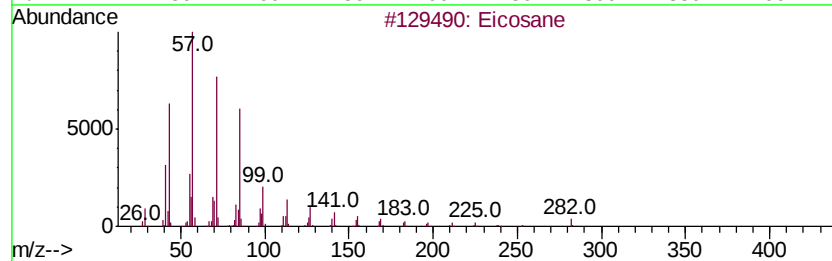
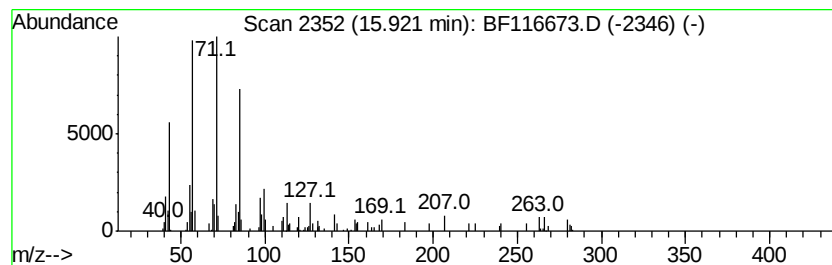
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	3.04 ng	116100	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	93
2		Hexadecane	226	C16H34	000544-76-3	91
3		Triacontane	422	C30H62	000638-68-6	87
4		6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	86
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083019\
Data File : BF116673.D
Acq On : 31 Aug 2019 1:58
Operator : HP/JU
Sample : K4517-12
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T4-S-D1-D4

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
unknown6.62	6.62	69.7	ng	2258650	1	6.85	648336	20.0
n-Hexadecanoic acid	11.89	5.8	ng	292876	4	11.36	1002220	20.0
Octadecanoic acid	12.67	2.1	ng	105521	4	11.36	1002220	20.0
1-Heneicosanol	13.83	8.8	ng	464869	5	13.99	1056440	20.0
Octadecane	14.47	2.4	ng	128504	5	13.99	1056440	20.0
2-methyloctacosane	14.77	3.0	ng	115338	6	15.44	764423	20.0
Azacyclotridecan-...	14.84	2.3	ng	87542	6	15.44	764423	20.0
Perylene	15.32	5.8	ng	219725	6	15.44	764423	20.0
Eicosane	15.92	3.0	ng	116100	6	15.44	764423	20.0