

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041119\
 Data File : BF113718.D
 Acq On : 11 Apr 2019 14:12
 Operator : JU/SJ
 Sample : K2358-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF040319.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	5.287	540	544	565	rBV	2025230	2370894	71.29%	8.164%
2	6.328	717	721	737	rBV	2219553	2557974	76.91%	8.808%
3	6.445	737	741	750	rVB	2768602	2495861	75.05%	8.594%
4	6.669	776	779	792	rVB	729179	708153	21.29%	2.438%
5	6.828	802	806	823	rBV	2176348	1976878	59.44%	6.807%
6	7.239	872	876	899	rBV	1514055	1619375	48.69%	5.576%
7	7.957	994	998	1007	rBV	782790	900708	27.08%	3.101%
8	8.022	1007	1009	1017	rVB2	23926	34093	1.03%	0.117%
9	9.027	1176	1180	1192	rBV	3245508	2987366	89.82%	10.286%
10	9.427	1244	1248	1257	rBV	289780	294742	8.86%	1.015%
11	9.704	1291	1295	1308	rVB	1170002	1056873	31.78%	3.639%
12	10.492	1425	1429	1444	rBV	1737048	1894313	56.96%	6.523%
13	11.186	1543	1547	1559	rBV	1215015	1271475	38.23%	4.378%
14	11.721	1635	1638	1646	rBV3	173712	220368	6.63%	0.759%
15	12.398	1750	1753	1764	rBV	142498	162211	4.88%	0.559%
16	12.504	1768	1771	1778	rBV	104849	155577	4.68%	0.536%
17	12.627	1787	1792	1800	rVB	132691	171596	5.16%	0.591%
18	12.768	1811	1816	1819	rBV	3375349	3325818	100.00%	11.452%
19	13.251	1893	1898	1904	rVB2	24191	36895	1.11%	0.127%
20	13.339	1908	1913	1915	rBV2	39364	42579	1.28%	0.147%
21	13.662	1965	1968	1973	rVB	59632	56599	1.70%	0.195%
22	13.745	1973	1982	1989	rBV4	108867	423951	12.75%	1.460%
23	13.821	1991	1995	2007	rVB	1162394	1334301	40.12%	4.594%
24	13.980	2018	2022	2026	rBV	149734	135263	4.07%	0.466%
25	14.286	2070	2074	2077	rVB	218360	210417	6.33%	0.725%
26	14.574	2120	2123	2128	rBV	274425	277657	8.35%	0.956%
27	14.845	2165	2169	2171	rBV	41479	54681	1.64%	0.188%
28	14.886	2172	2176	2183	rVB	310051	326420	9.81%	1.124%
29	15.174	2222	2225	2229	rVB	44776	44526	1.34%	0.153%
30	15.227	2229	2234	2247	rBV	1004275	1337988	40.23%	4.607%
31	15.621	2296	2301	2308	rVB	180547	251987	7.58%	0.868%
32	16.074	2373	2378	2388	rVB2	104356	186949	5.62%	0.644%
33	16.603	2462	2468	2477	rVB5	51151	117164	3.52%	0.403%

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ClientSampleId :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

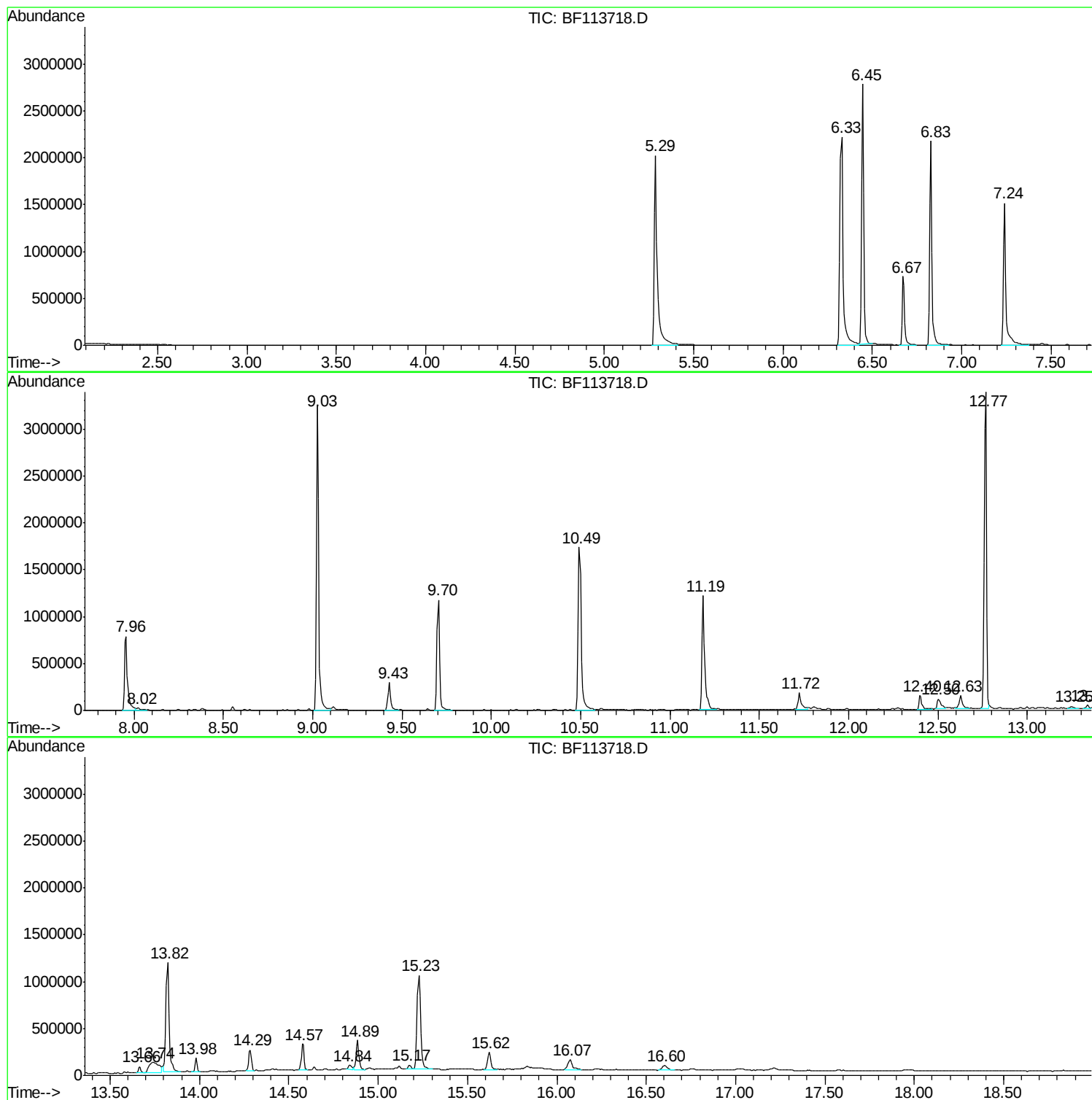
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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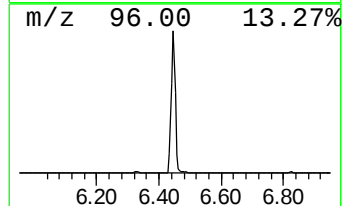
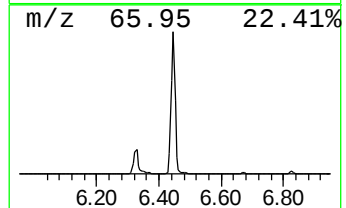
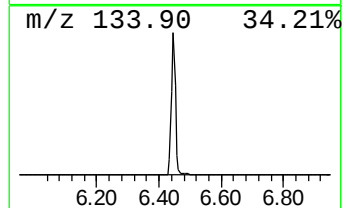
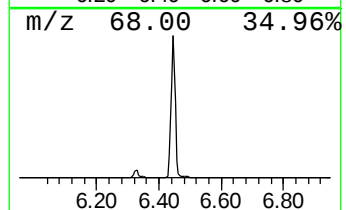
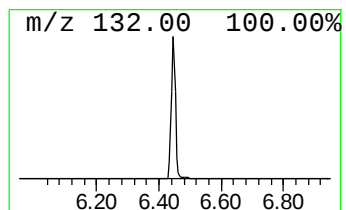
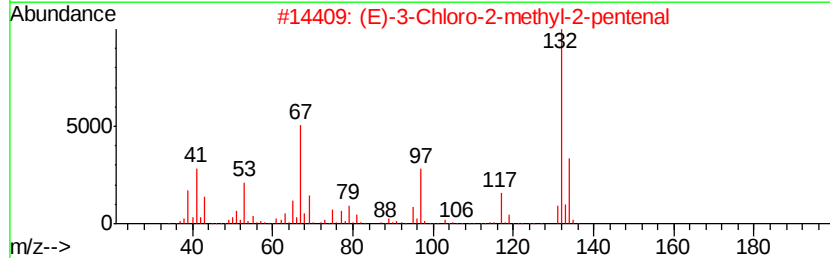
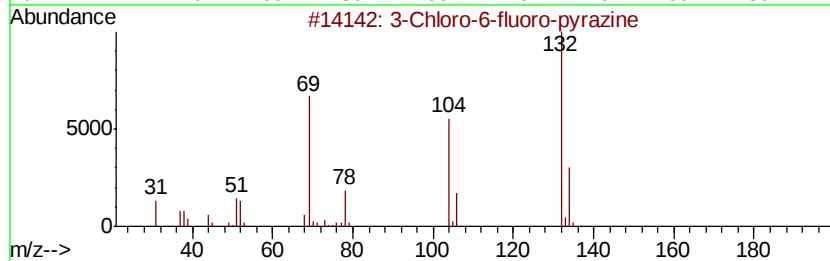
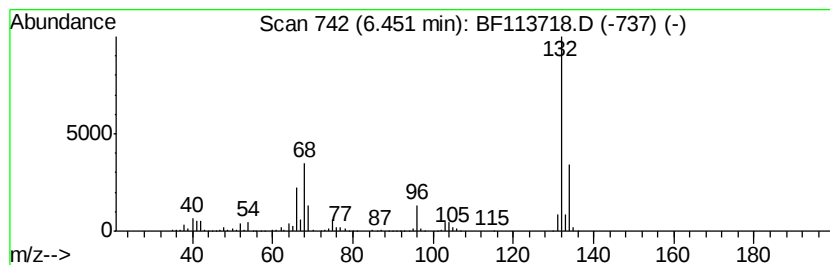
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	70.49 ng	2495860	1,4-Dichlorobenzene-d4	6.67

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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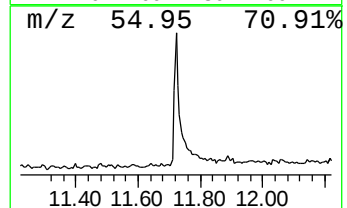
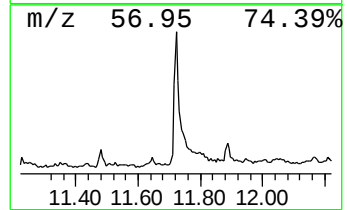
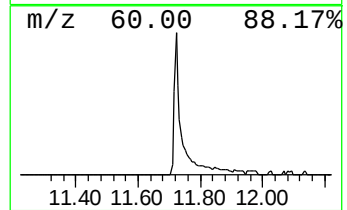
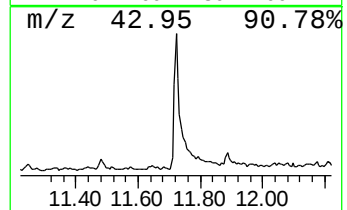
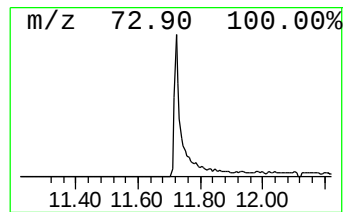
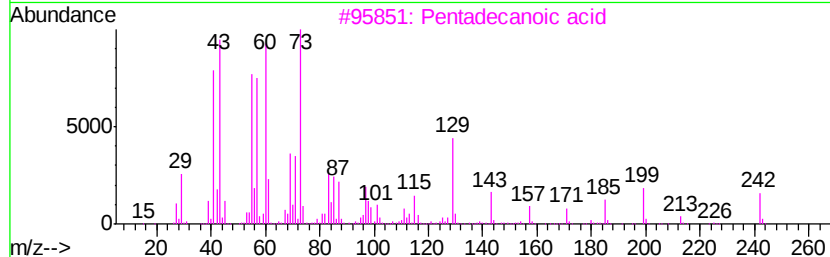
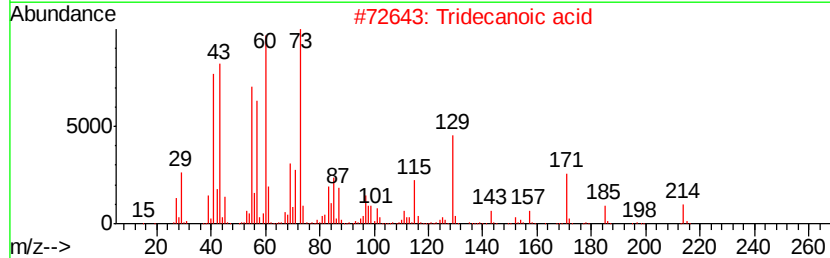
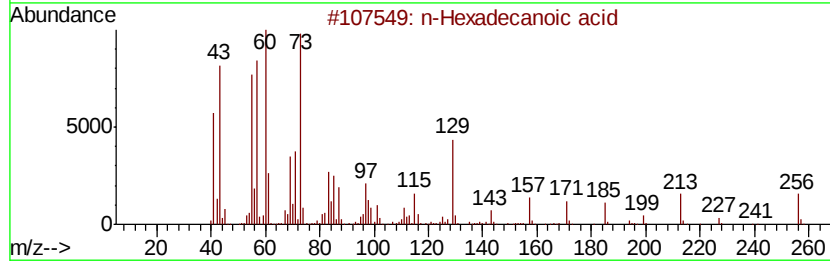
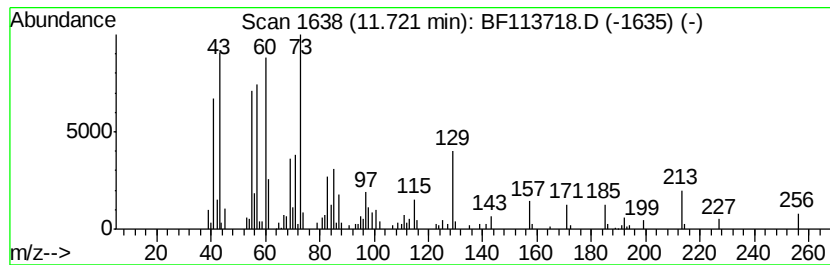
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BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.72	3.47 ng	220368	Phenanthrene-d10		11.19
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



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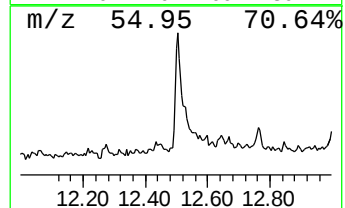
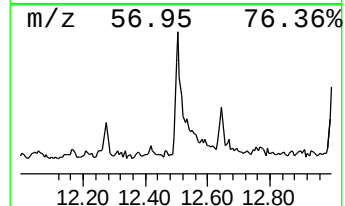
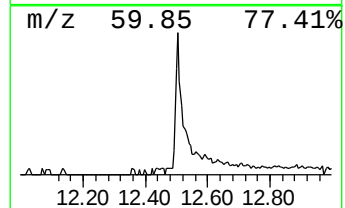
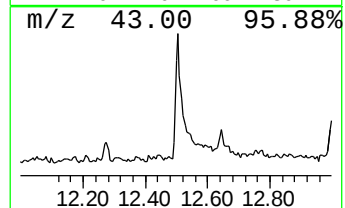
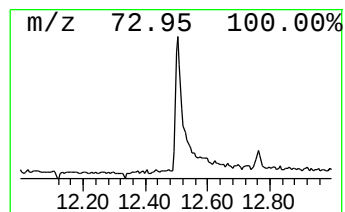
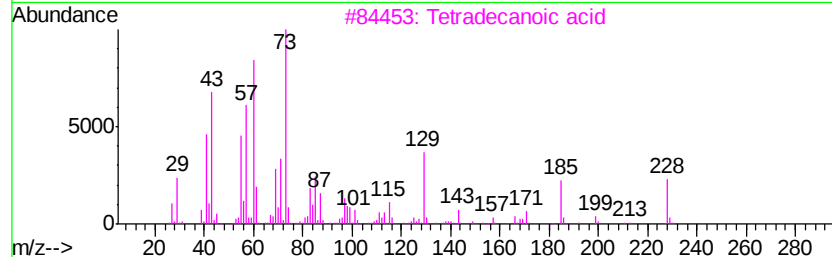
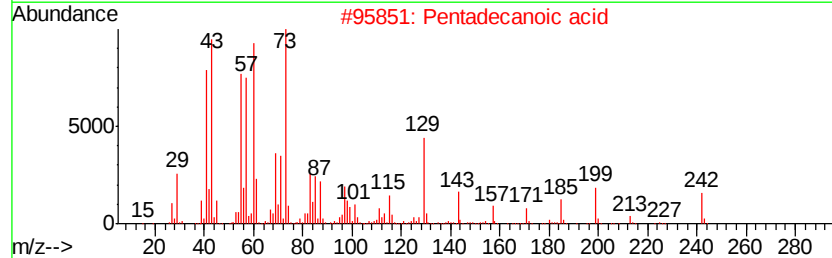
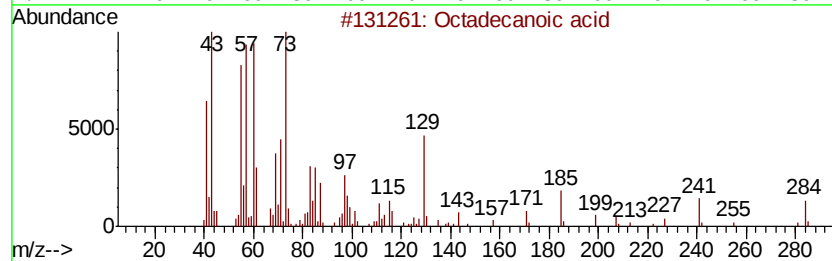
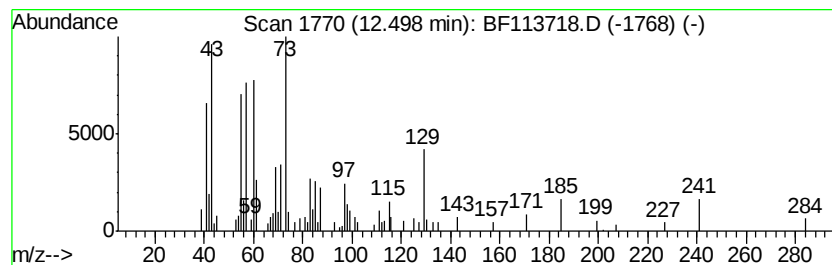
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.50	2.33 ng	155577	Chrysene-d12		13.82
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Undecanoic acid	186	C11H22O2	000112-37-8	70



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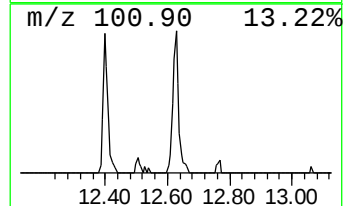
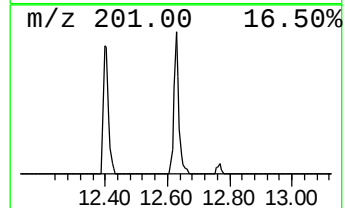
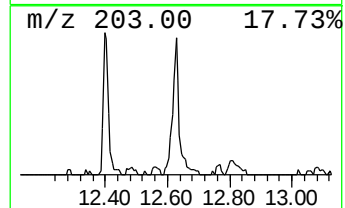
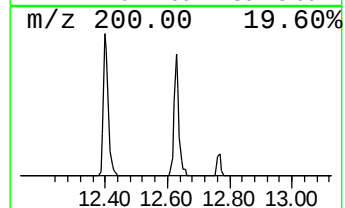
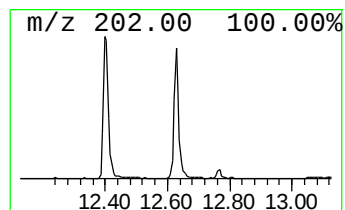
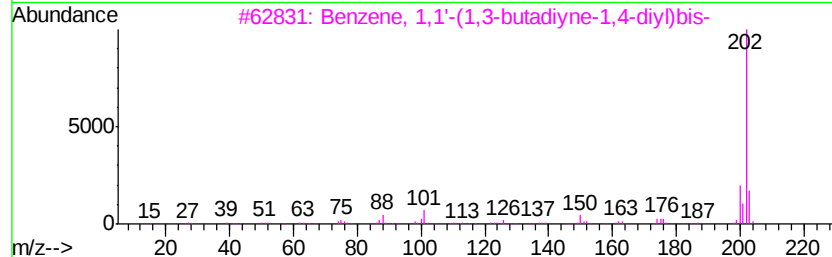
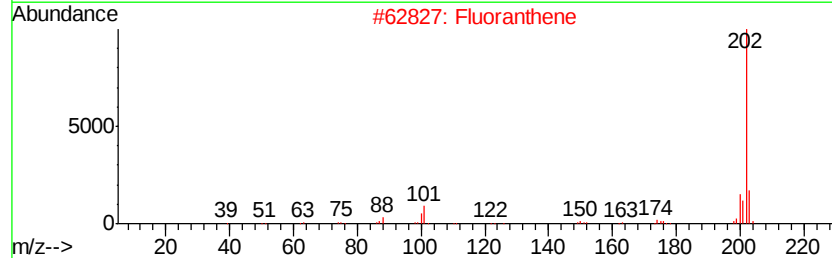
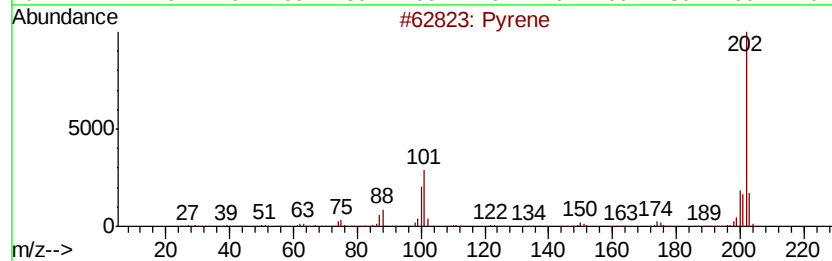
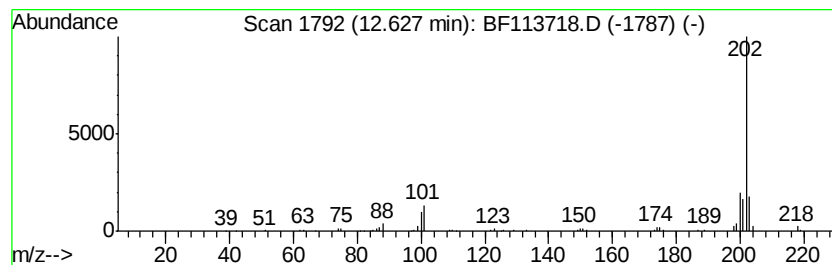
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	2.57 ng	171596	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene	202	C16H10	000129-00-0	95
2		Fluoranthene	202	C16H10	000206-44-0	91
3		Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	59
4		l-Leucyl-l-leucine, N,N'-dimethy...	458	C24H46N2O6	1000328-59-2	33
5		5H-1,2,4-Triazino[5,6-b]indole-3...	202	C9H6N4S	028668-95-3	9



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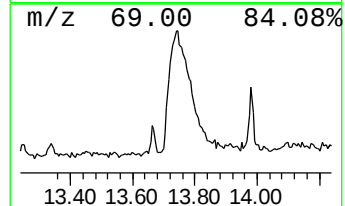
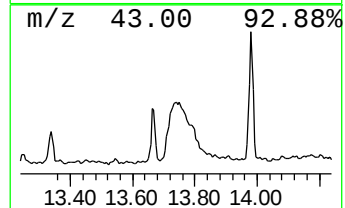
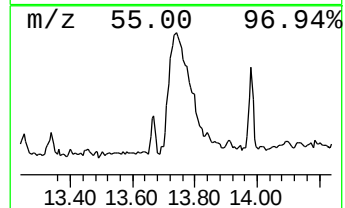
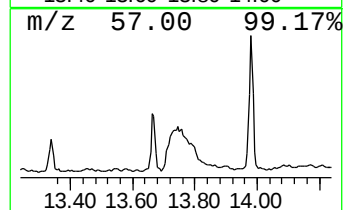
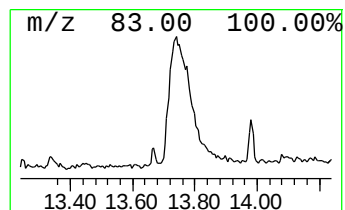
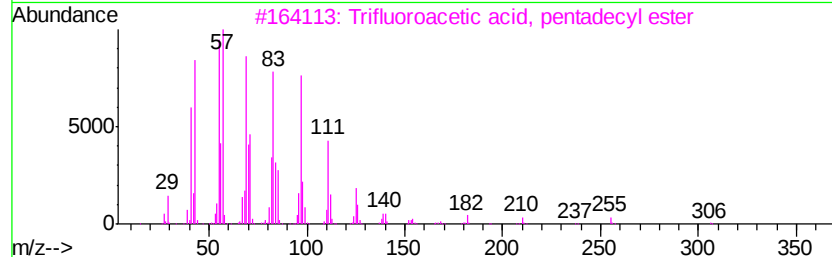
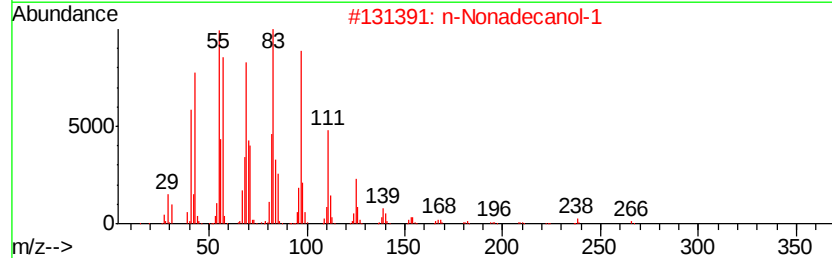
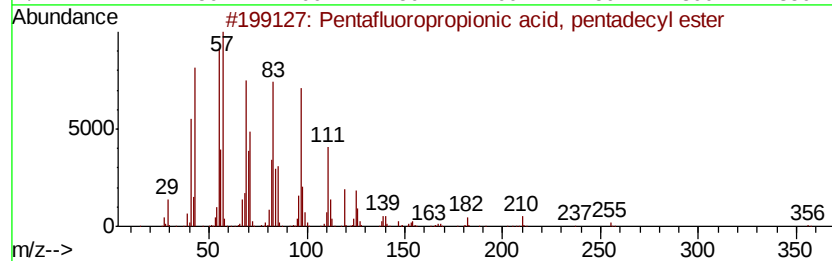
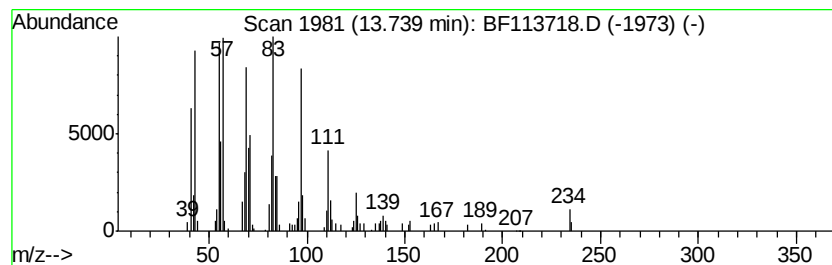
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	6.35 ng	423951	Chrysene-d12	13.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	95
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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ALS Vial : 5 Sample Multiplier: 1

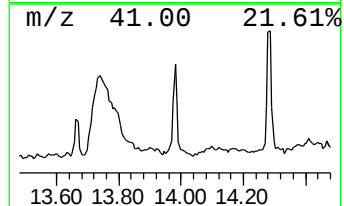
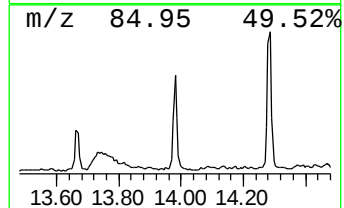
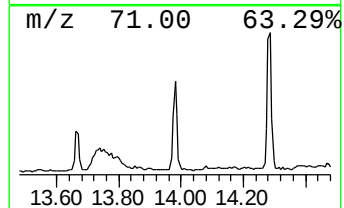
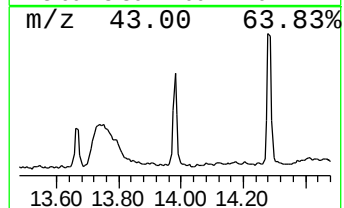
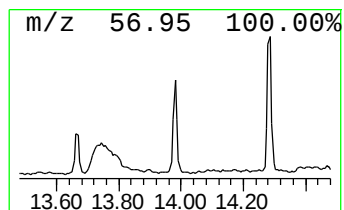
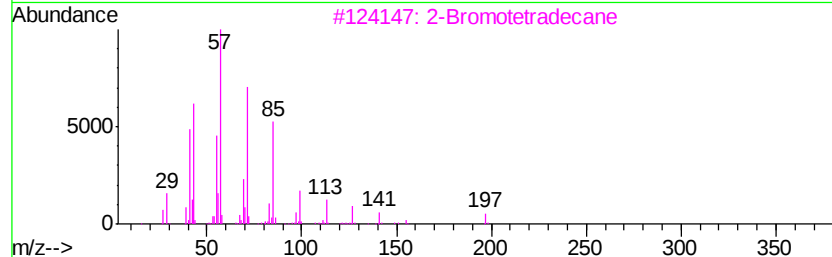
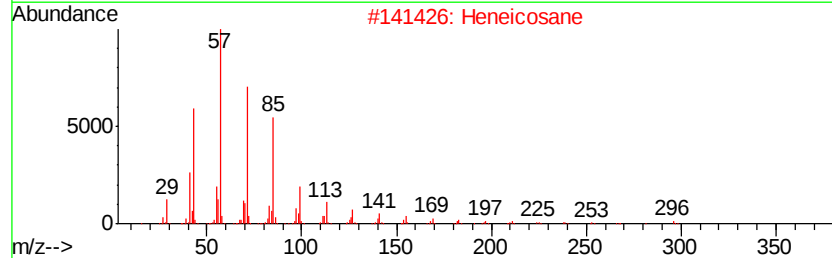
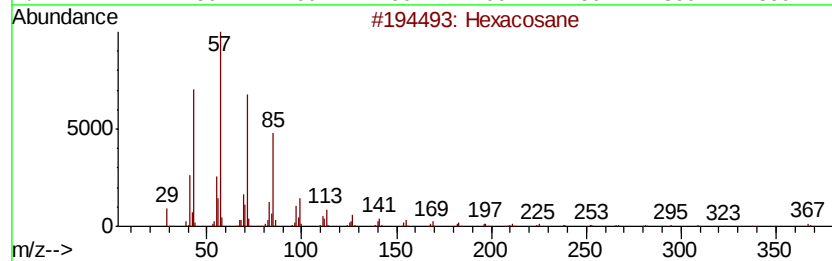
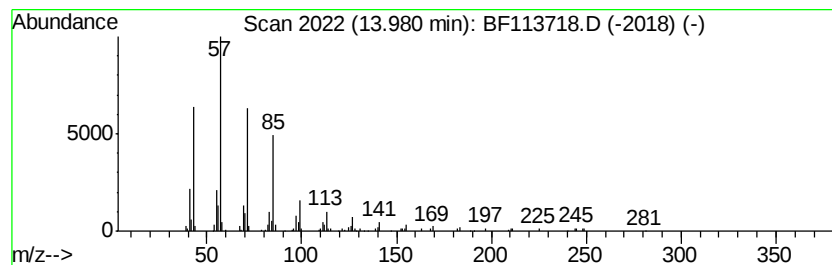
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.98	2.03 ng	135263	Chrysene-d12		13.82	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	90
2	Heneicosane		296	C21H44	000629-94-7	90
3	2-Bromotetradecane		276	C14H29Br	074036-95-6	87
4	Octadecane		254	C18H38	000593-45-3	87
5	Hexadecane		226	C16H34	000544-76-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041119\
Data File : BF113718.D
Acq On : 11 Apr 2019 14:12
Operator : JU/SJ
Sample : K2358-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-9

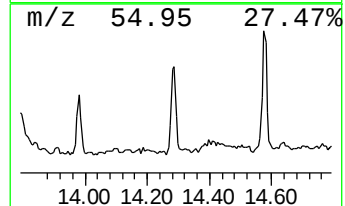
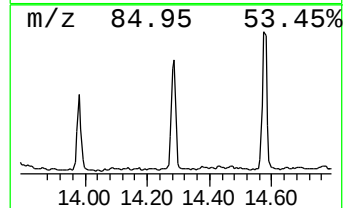
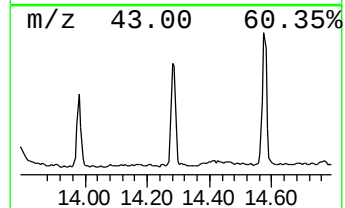
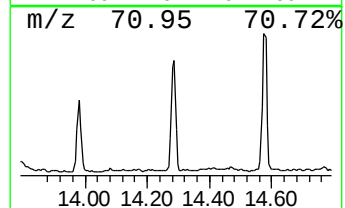
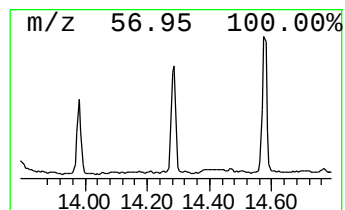
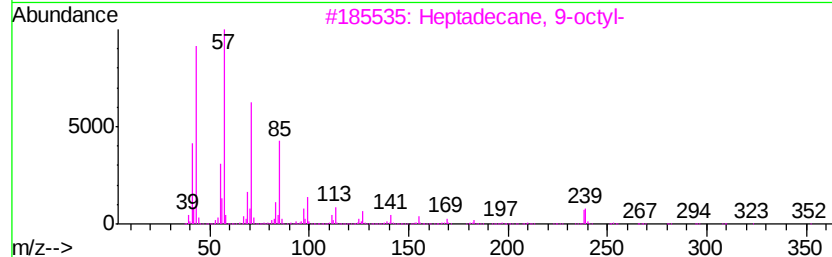
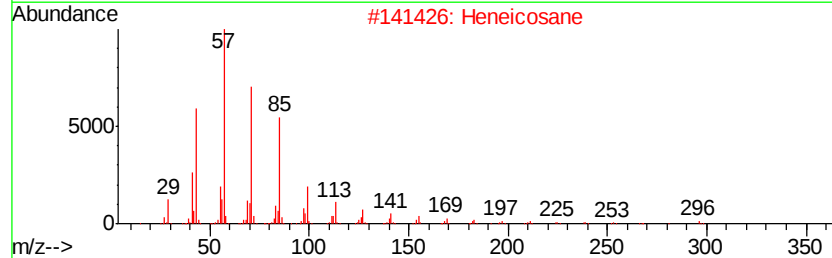
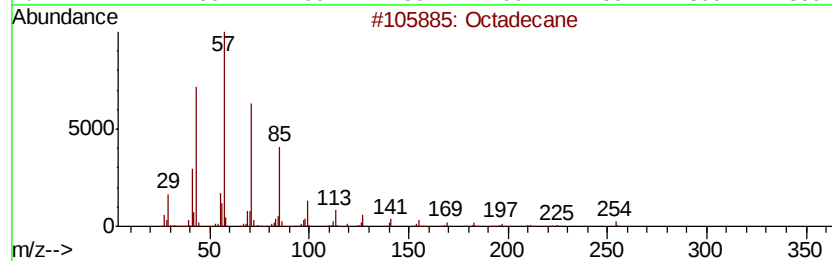
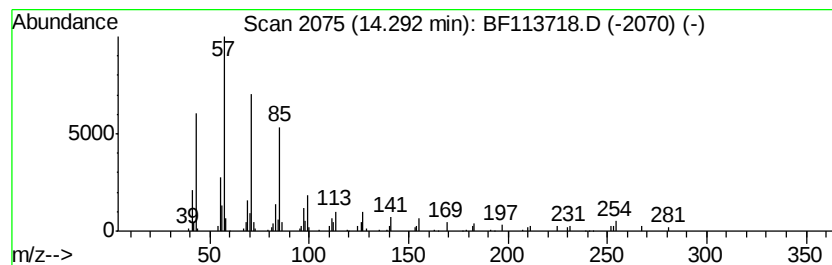
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	3.15 ng	210417	Chrysene-d12	13.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	93
2	Heneicosane		296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
4	Hexacosane		366	C26H54	000630-01-3	91
5	Eicosane, 2-methyl-		296	C21H44	001560-84-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041119\
Data File : BF113718.D
Acq On : 11 Apr 2019 14:12
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Sample : K2358-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

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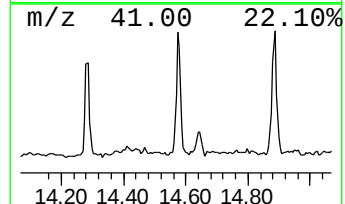
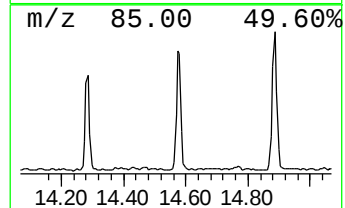
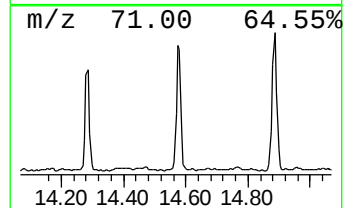
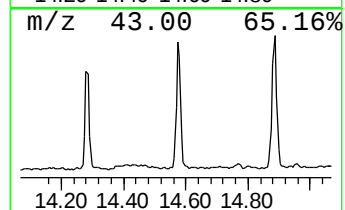
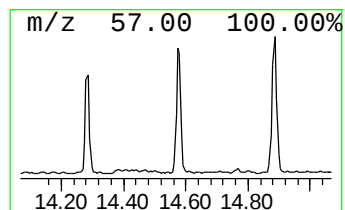
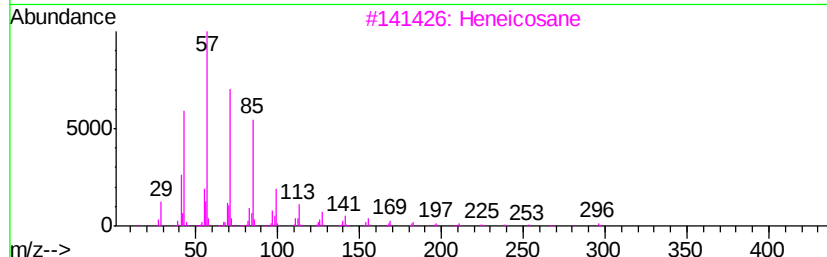
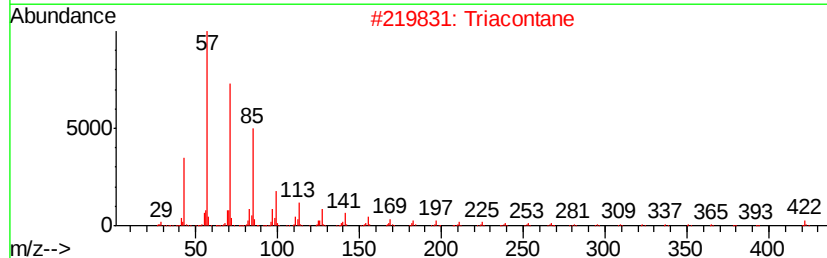
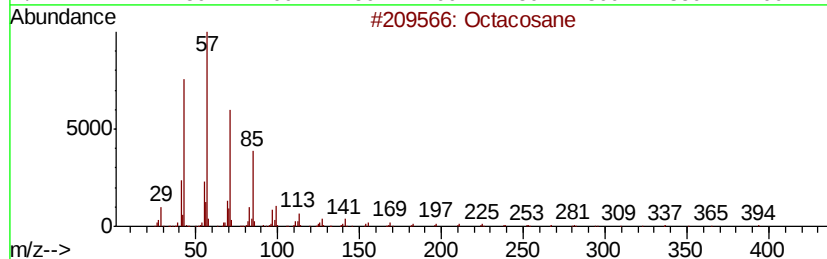
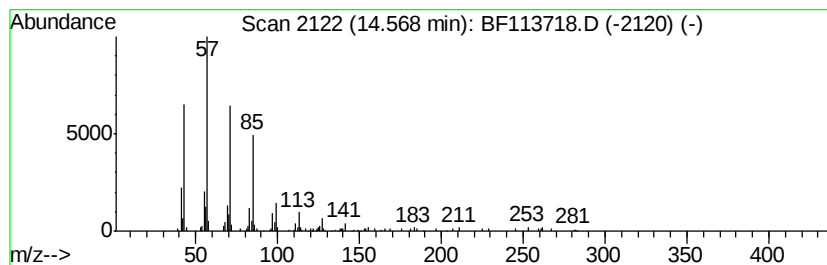
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	4.15 ng	277657	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041119\
 Data File : BF113718.D
 Acq On : 11 Apr 2019 14:12
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 Sample : K2358-07
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

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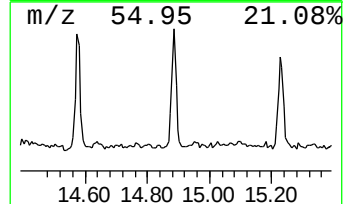
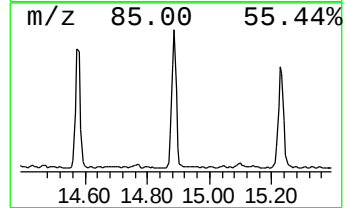
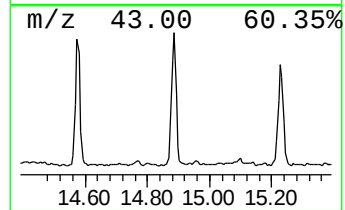
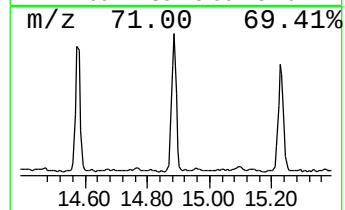
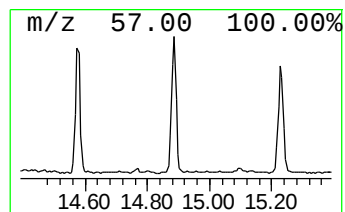
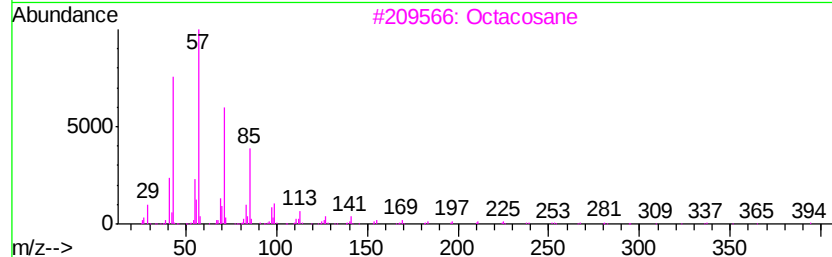
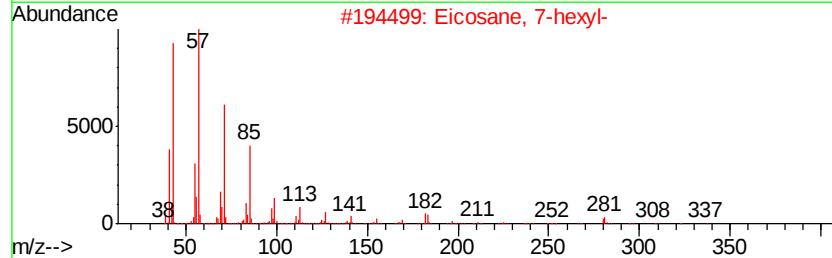
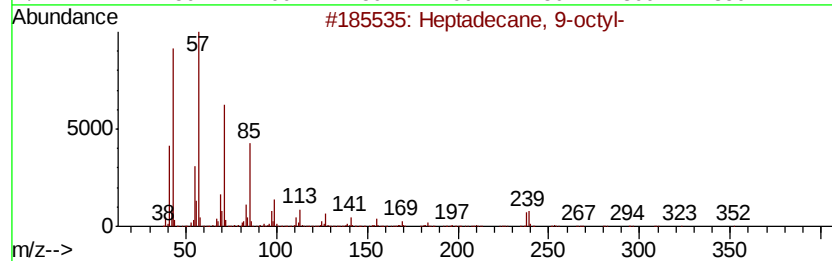
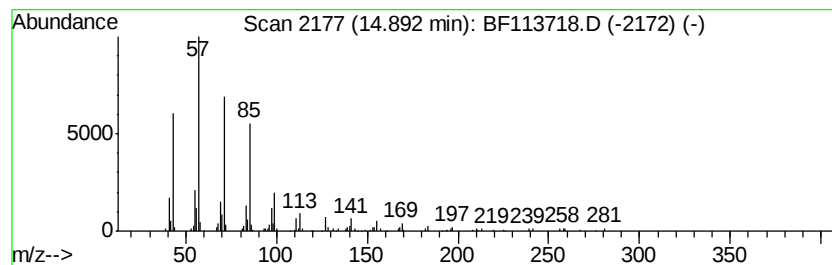
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	4.88 ng	326420	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
3		Octacosane	394	C28H58	000630-02-4	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041119\
Data File : BF113718.D
Acq On : 11 Apr 2019 14:12
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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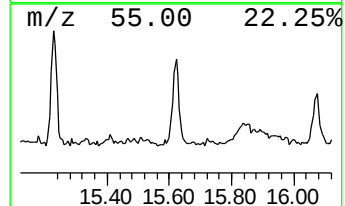
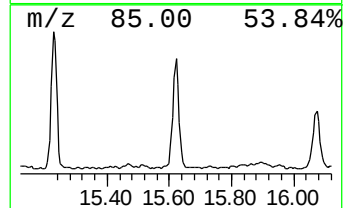
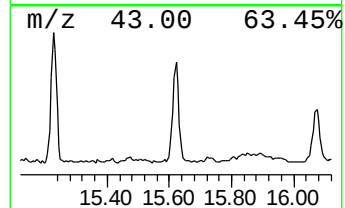
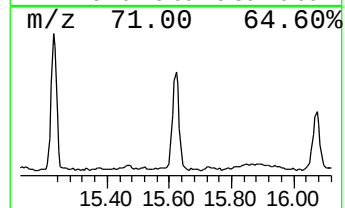
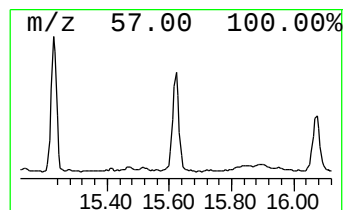
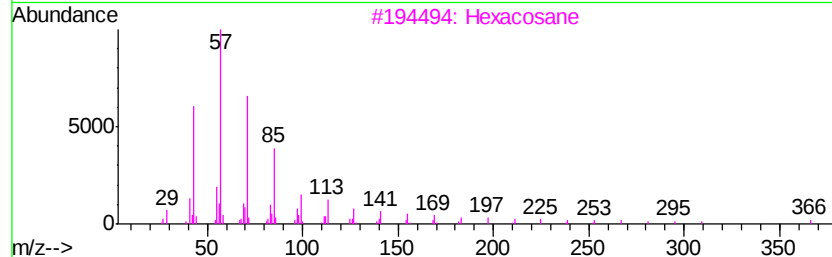
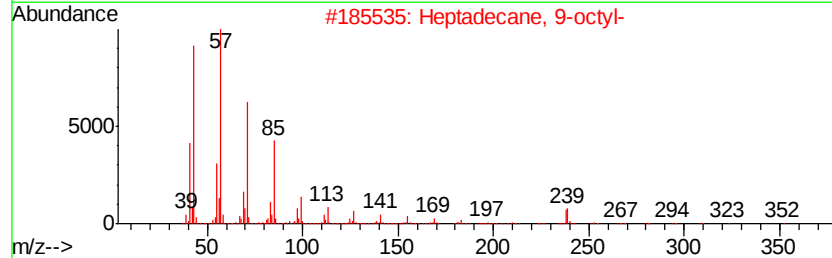
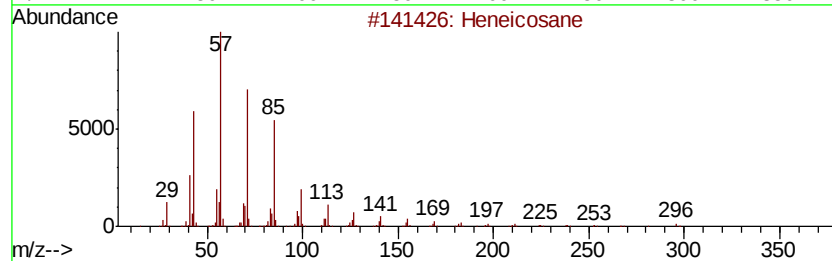
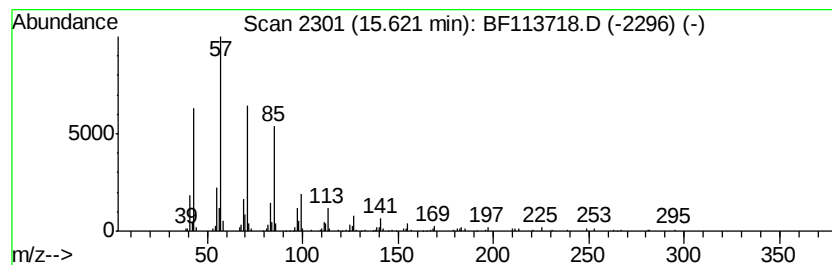
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane, 7-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	3.77 ng	251987	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	86
5		Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF041119\
Data File : BF113718.D
Acq On : 11 Apr 2019 14:12
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Sample : K2358-07
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ALS Vial : 5 Sample Multiplier: 1

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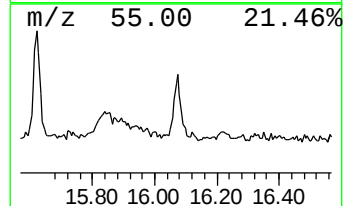
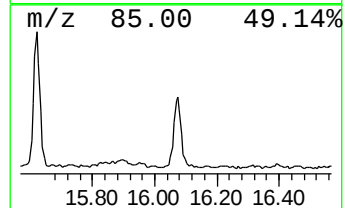
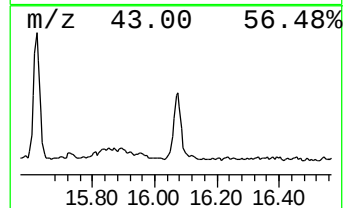
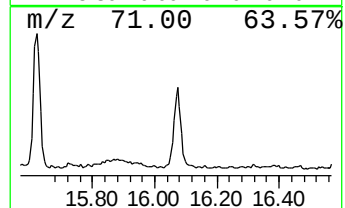
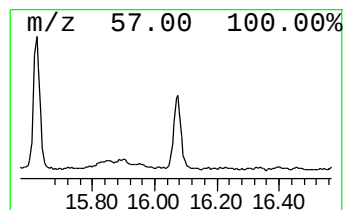
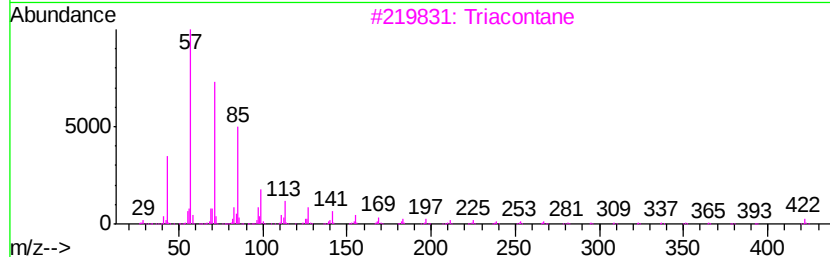
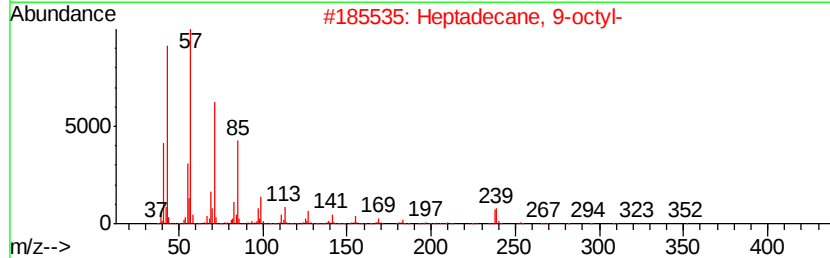
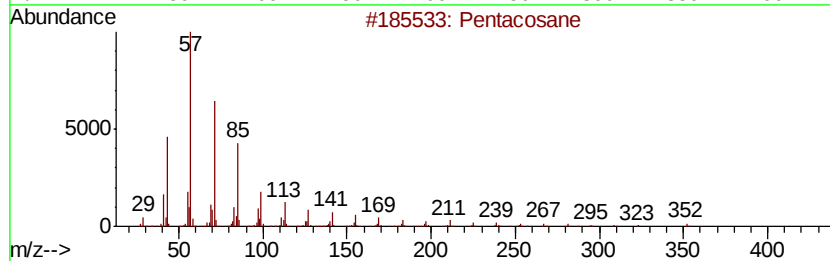
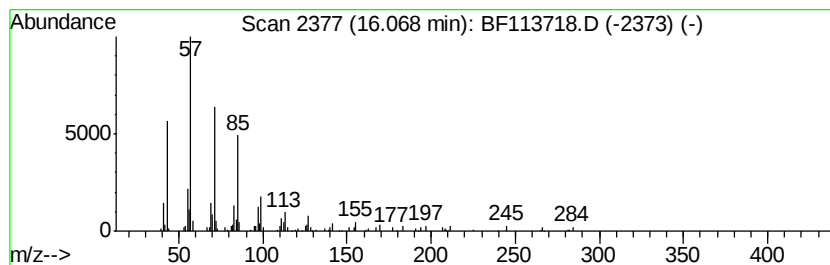
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	2.79 ng	186949	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		triacontane	422	C30H62	000638-68-6	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	90
5		Hentriacontane	437	C31H64	000630-04-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041119\
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Acq On : 11 Apr 2019 14:12
Operator : JU/SJ
Sample : K2358-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic acid	11.72	3.5	ng	220368	4	11.19	1271480	20.0
Octadecanoic acid	12.50	2.3	ng	155577	5	13.82	1334300	20.0
Benzene, 1,1'-(1,...	12.63	2.6	ng	171596	5	13.82	1334300	20.0
Pentafluoropropio...	13.74	6.3	ng	423951	5	13.82	1334300	20.0
Hexacosane	13.98	2.0	ng	135263	5	13.82	1334300	20.0
Octadecane	14.29	3.1	ng	210417	5	13.82	1334300	20.0
triacontane	14.57	4.2	ng	277657	6	15.23	1337990	20.0
Heptadecane, 9-oc...	14.89	4.9	ng	326420	6	15.23	1337990	20.0
Eicosane, 7-hexyl-	15.62	3.8	ng	251987	6	15.23	1337990	20.0
Pentacosane	16.07	2.8	ng	186949	6	15.23	1337990	20.0