

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
 Data File : BF112957.D
 Acq On : 11 Mar 2019 16:25
 Operator : JU/SJ
 Sample : K1785-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SD4-0.0-0.5

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-BF022719.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	5.334	548	552	556	rBV	3220522	3421876	76.54%	8.483%
2	6.369	722	728	738	rBV	3546482	3791078	84.80%	9.398%
3	6.498	745	750	753	rBV	4085913	3668901	82.07%	9.095%
4	6.728	786	789	793	rBV	1105158	877068	19.62%	2.174%
5	6.887	812	816	819	rBV	3223068	2692352	60.22%	6.674%
6	7.140	855	859	869	rVB	30246	45028	1.01%	0.112%
7	7.287	879	884	897	rBV	2266879	2341825	52.38%	5.805%
8	8.010	1003	1007	1014	rBV	1111812	1065923	23.84%	2.642%
9	9.086	1186	1190	1199	rBV	3887028	3652943	81.71%	9.055%
10	9.481	1253	1257	1267	rBV	239366	253024	5.66%	0.627%
11	9.763	1298	1305	1309	rBV	1346952	1344475	30.07%	3.333%
12	10.545	1433	1438	1450	rBV	3139052	3082621	68.95%	7.642%
13	11.239	1552	1556	1571	rVB	1546852	1583577	35.42%	3.926%
14	11.716	1631	1637	1639	rBV3	83613	111262	2.49%	0.276%
15	11.775	1644	1647	1657	rVV	554324	687135	15.37%	1.703%
16	11.851	1657	1660	1667	rVV2	117820	149379	3.34%	0.370%
17	11.922	1669	1672	1676	rVV	237702	204840	4.58%	0.508%
18	12.445	1757	1761	1763	rBV	115697	131495	2.94%	0.326%
19	12.480	1764	1767	1769	rBV2	87287	96388	2.16%	0.239%
20	12.557	1777	1780	1793	rVV	262449	433404	9.69%	1.074%
21	12.669	1797	1799	1804	rVB	118245	113963	2.55%	0.283%
22	12.822	1820	1825	1841	rVB	4235668	4470504	100.00%	11.082%
23	13.727	1973	1979	1992	rBV3	132991	239369	5.35%	0.593%
24	13.863	1995	2002	2015	rVB	1961201	2070359	46.31%	5.132%
25	14.045	2029	2033	2037	rBV	67333	64409	1.44%	0.160%
26	14.345	2081	2084	2091	rBV	131129	124718	2.79%	0.309%
27	14.639	2130	2134	2139	rBV	190726	199278	4.46%	0.494%
28	14.868	2169	2173	2181	rBV	59985	124904	2.79%	0.310%
29	14.957	2184	2188	2192	rBV	248428	280812	6.28%	0.696%
30	15.204	2227	2230	2235	rVB	44978	60164	1.35%	0.149%
31	15.268	2235	2241	2245	rBV	1345578	1712098	38.30%	4.244%
32	15.310	2245	2248	2255	rVB	273637	381555	8.53%	0.946%
33	15.715	2312	2317	2323	rBV	247663	360473	8.06%	0.894%
34	16.186	2392	2397	2407	rVB	142864	255955	5.73%	0.634%

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

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.733	2486	2490	2495	rVB2	53674	95127	2.13%	0.236%
36	16.798	2496	2501	2511	rVV8	78066	152104	3.40%	0.377%

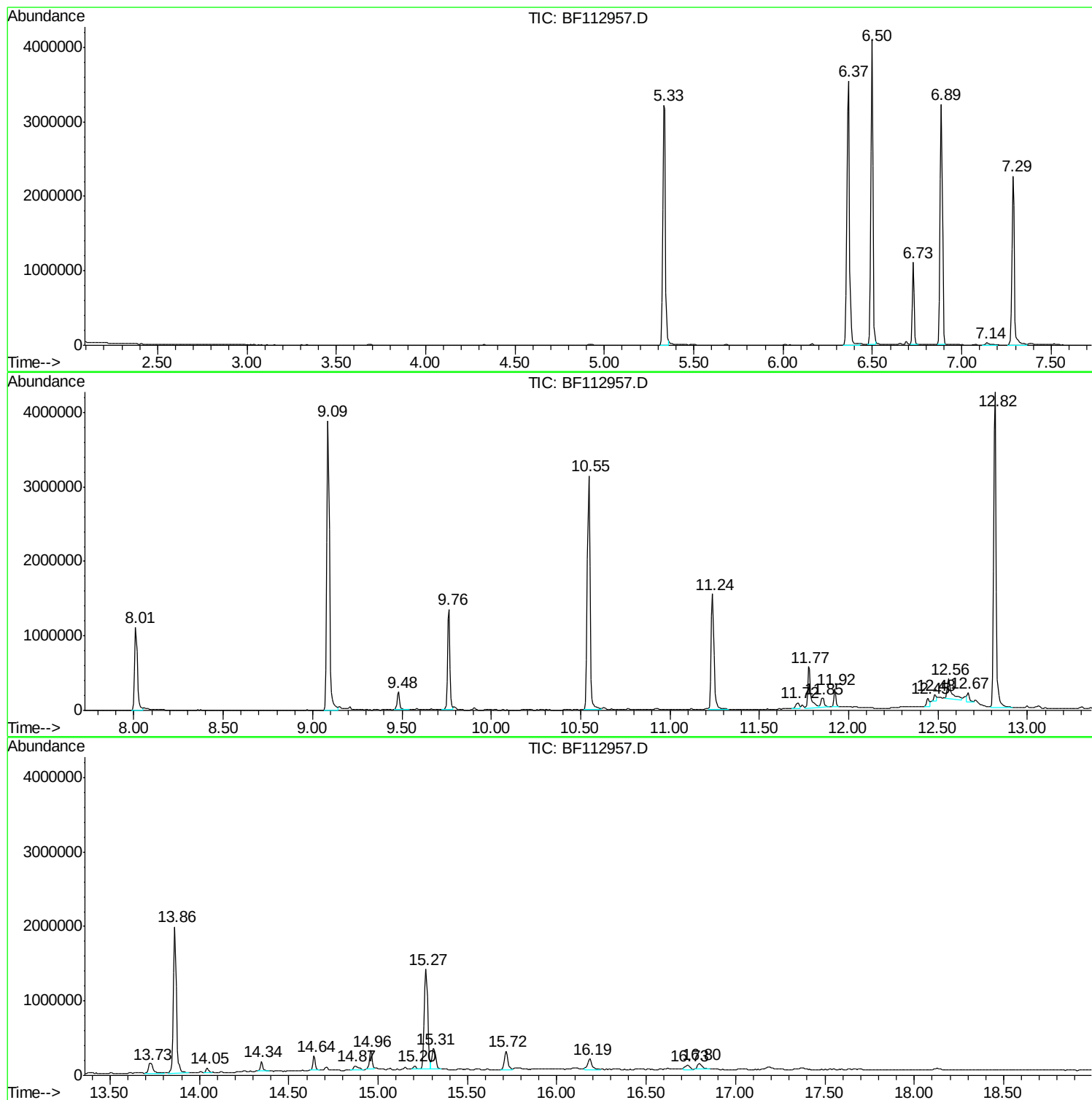
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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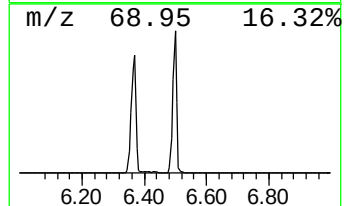
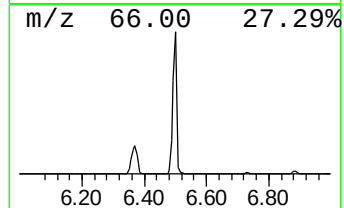
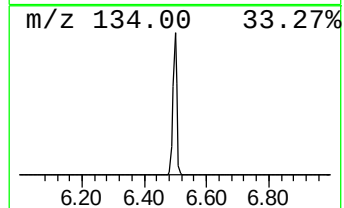
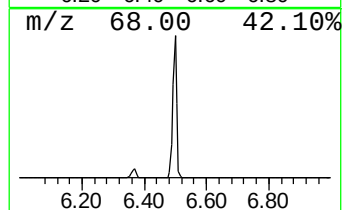
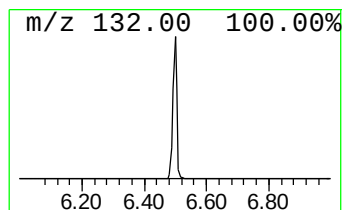
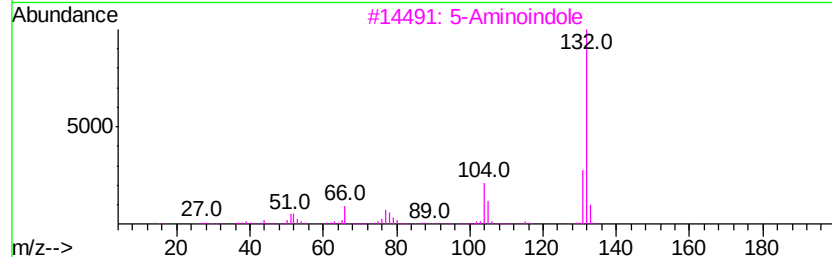
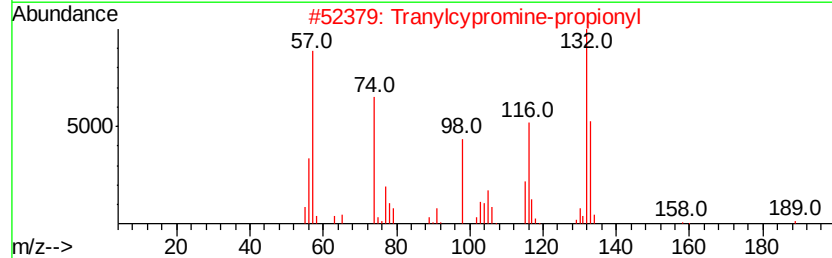
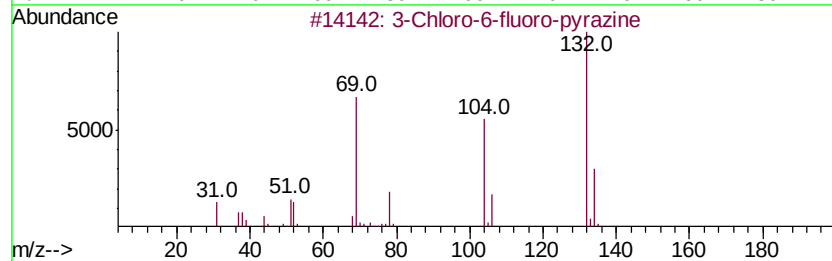
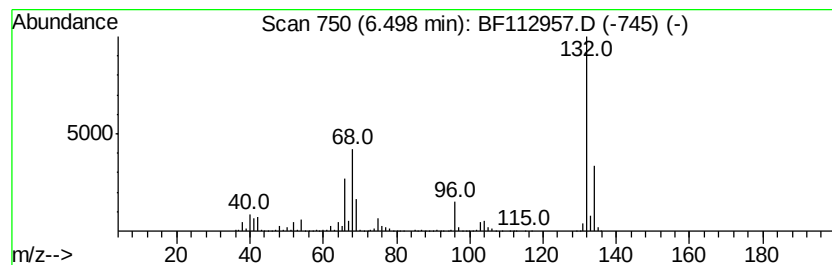
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	83.66 ng	3668900	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12



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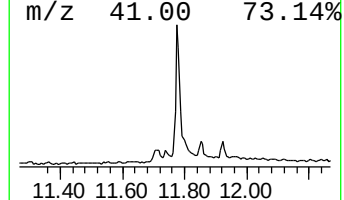
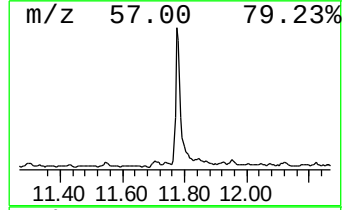
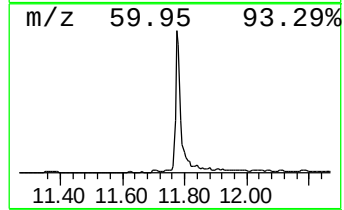
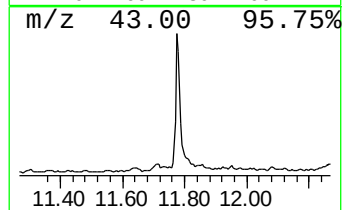
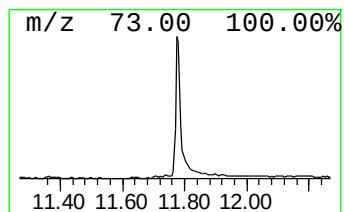
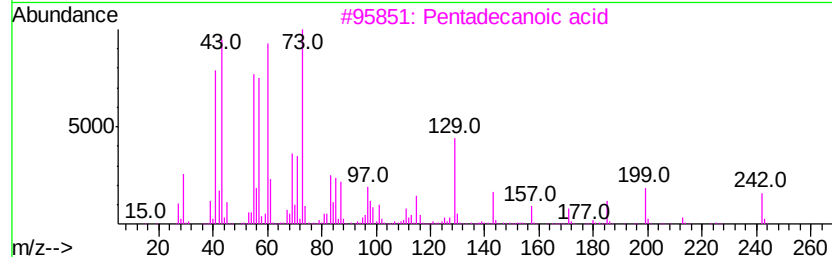
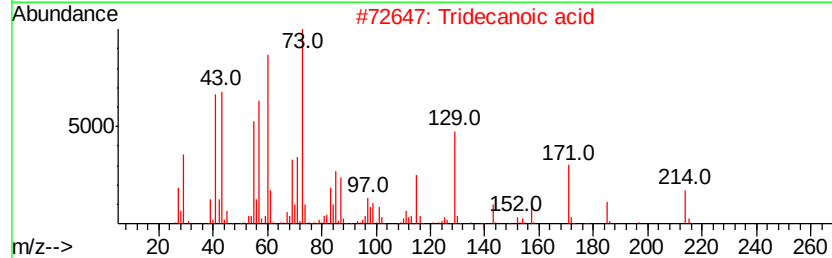
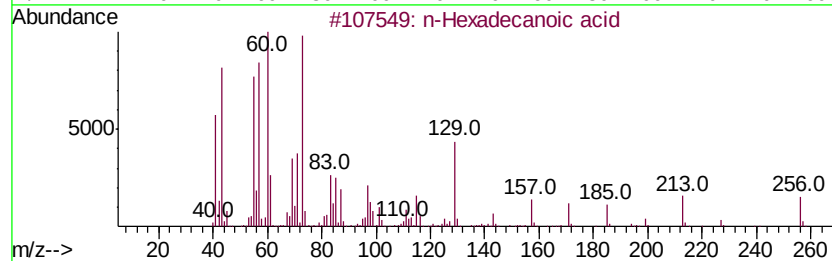
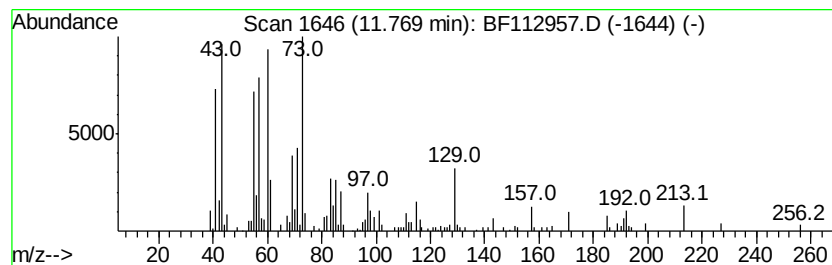
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	8.68 ng	687135	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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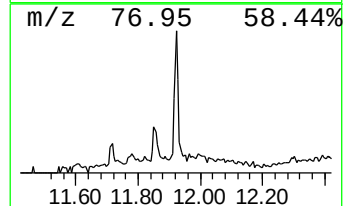
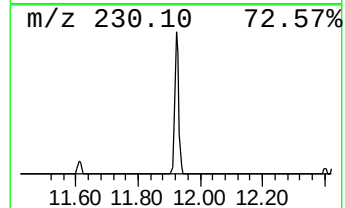
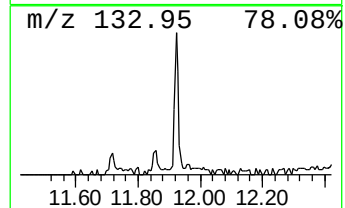
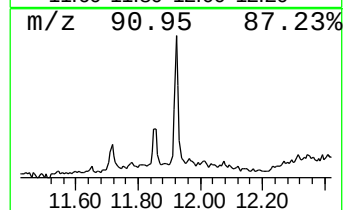
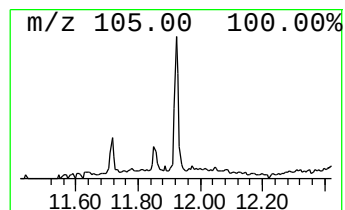
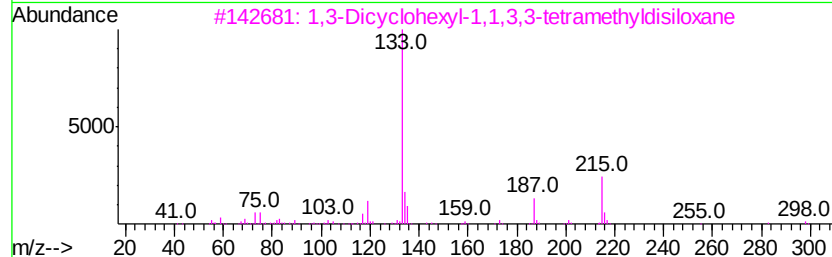
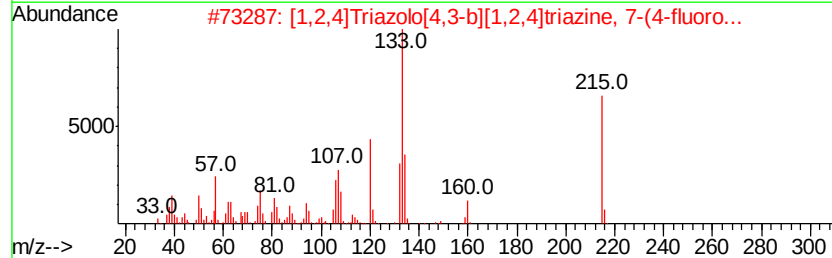
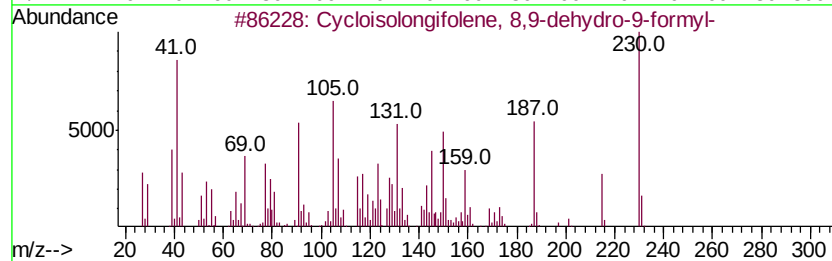
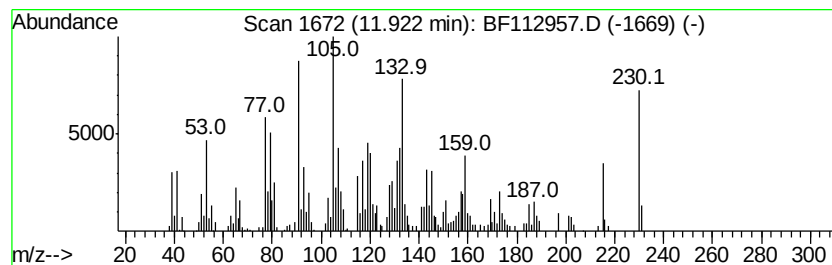
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.92 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.92	2.59 ng	204840	Phenanthrene-d10		11.24	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cycloisolongifolene, 8,9-dehydro...	230	C16H22O	059820-24-5	25
2		[1,2,4]Triazolo[4,3-b][1,2,4]tri...	215	C10H6FN5	1000338-28-8	22
3		1,3-Dicyclohexyl-1,1,3,3-tetrame...	298	C16H34OSi2	062399-01-3	14
4		1,5-Heptadiyne	92	C7H8	000764-56-7	14
5		Trihydroxyphenethylamine, 3,4,5-	169	C8H11NO3	001927-04-4	14



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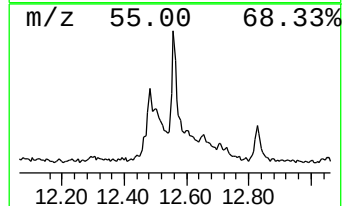
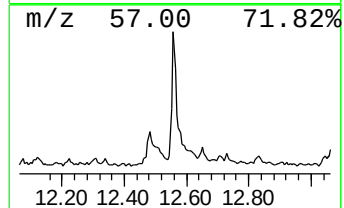
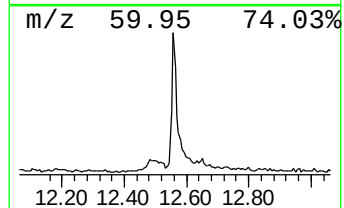
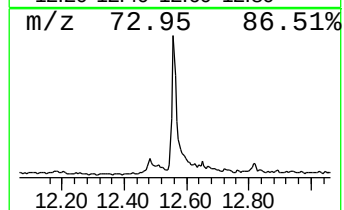
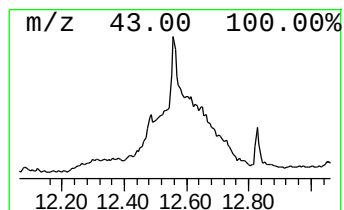
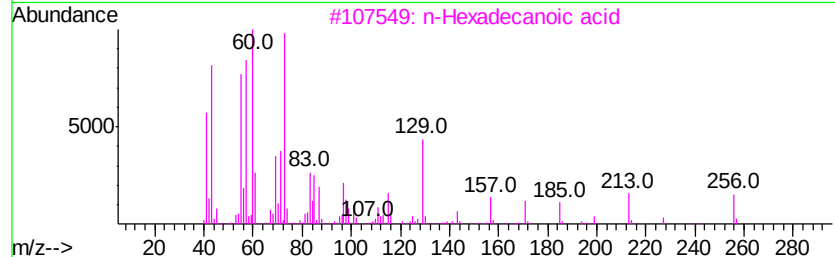
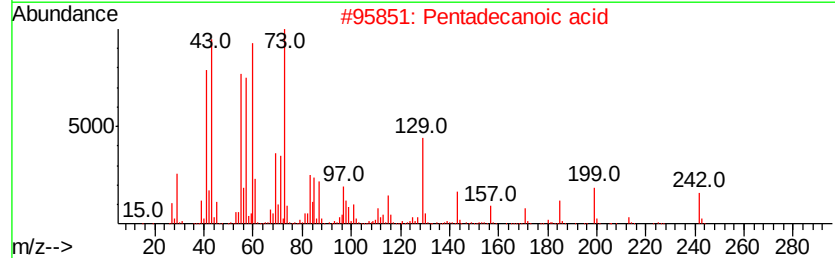
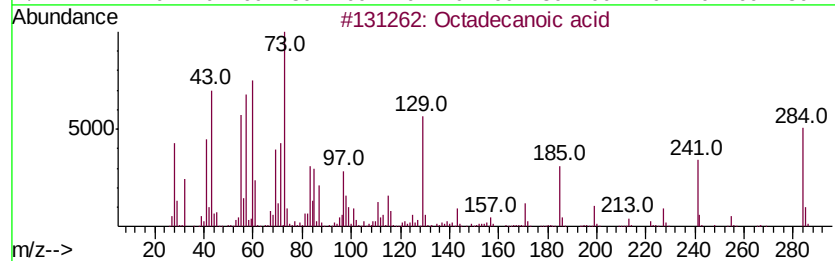
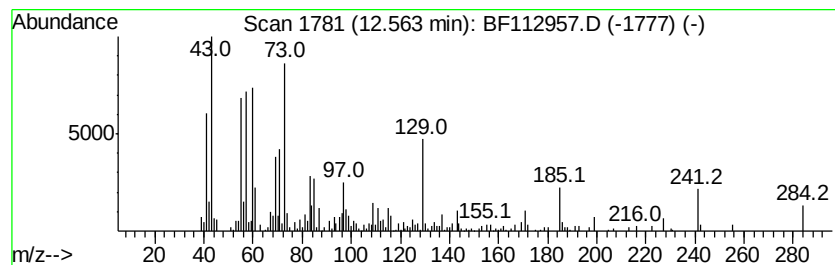
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.56	4.19 ng	433404	Chrysene-d12	13.86	
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	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83



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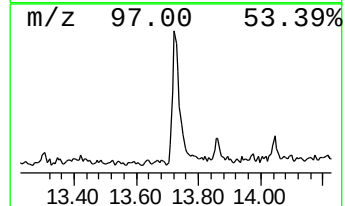
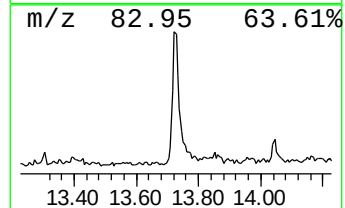
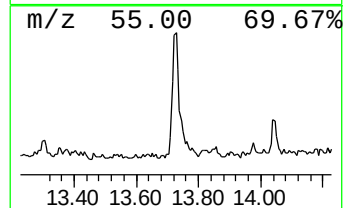
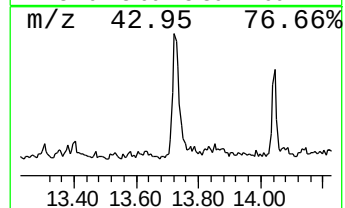
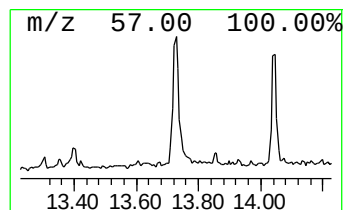
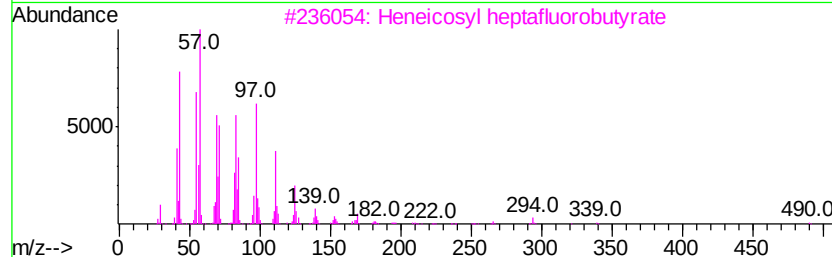
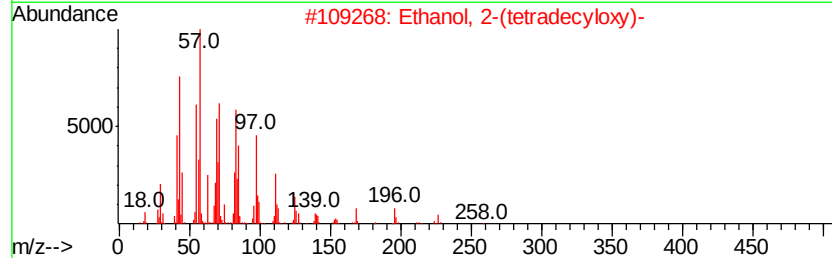
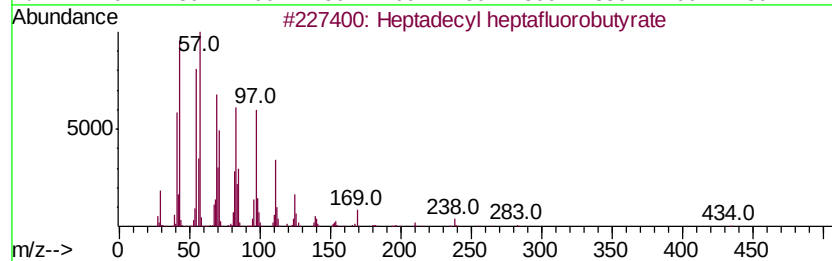
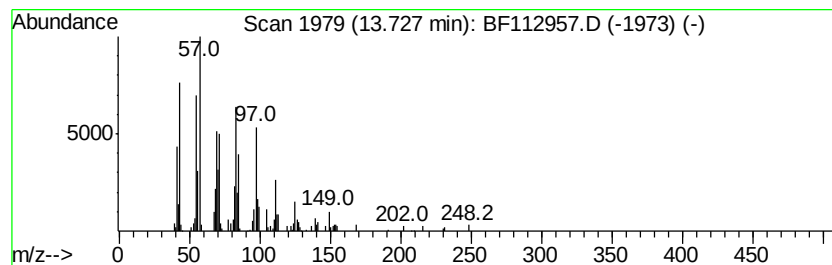
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.73	2.31 ng	239369	Chrysene-d12		13.86	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	90
4		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
5		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112957.D
Acq On : 11 Mar 2019 16:25
Operator : JU/SJ
Sample : K1785-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD4-0.0-0.5

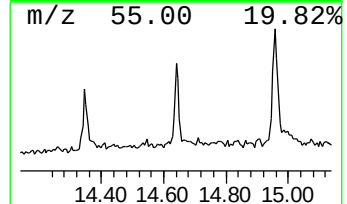
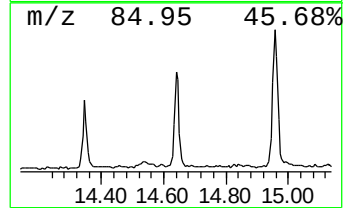
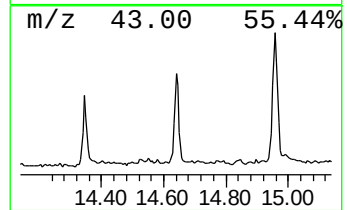
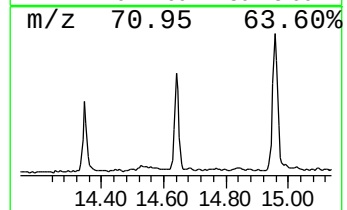
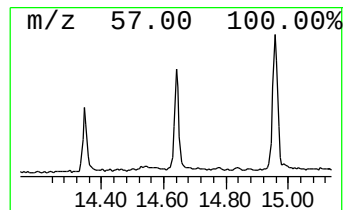
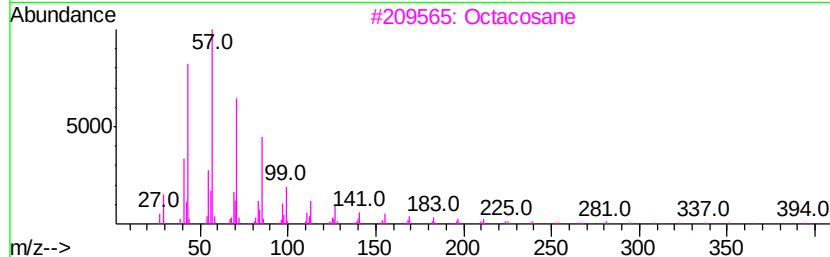
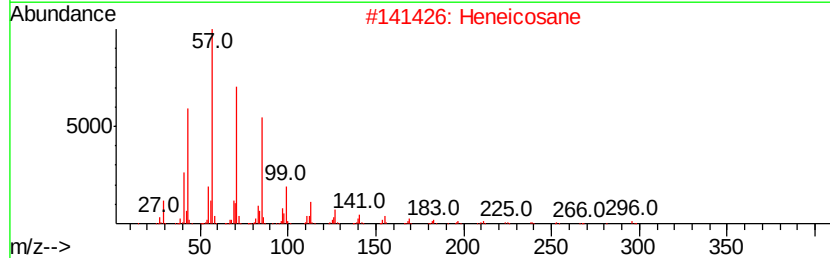
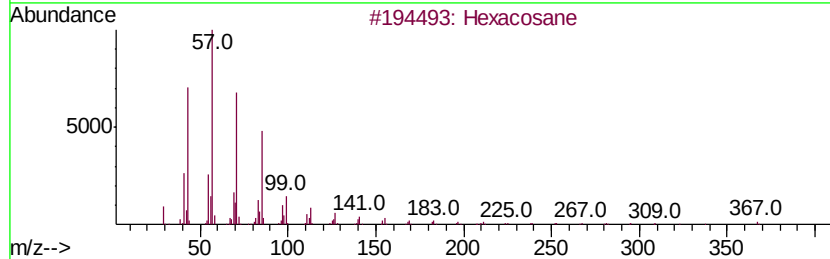
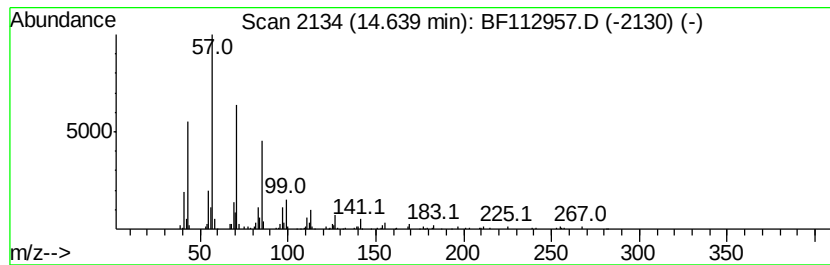
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.33 ng	199278	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5		triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112957.D
Acq On : 11 Mar 2019 16:25
Operator : JU/SJ
Sample : K1785-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

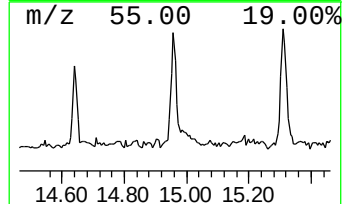
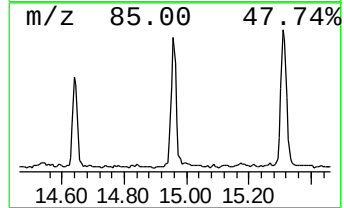
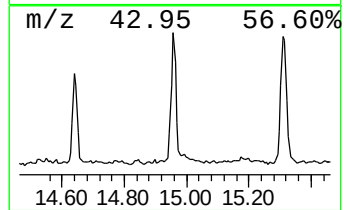
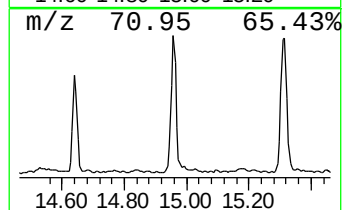
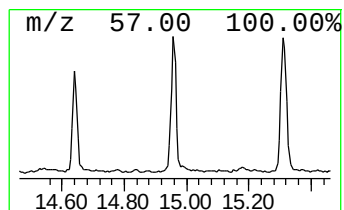
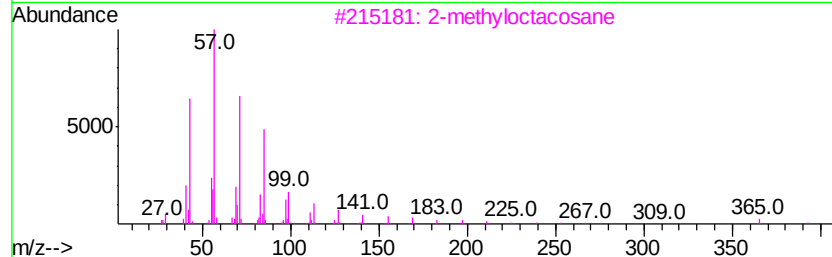
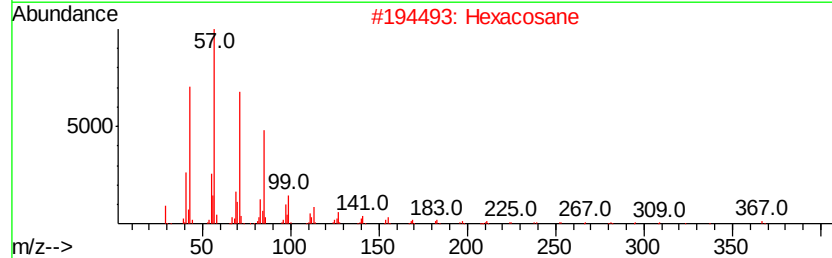
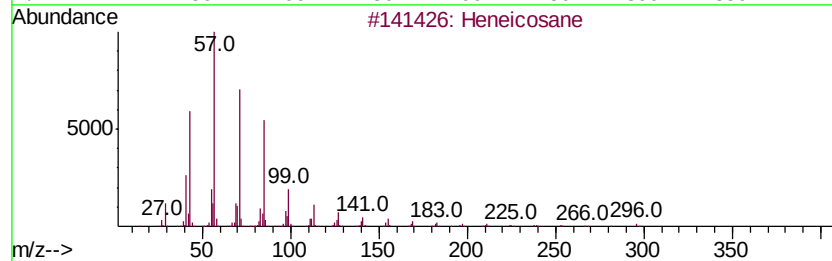
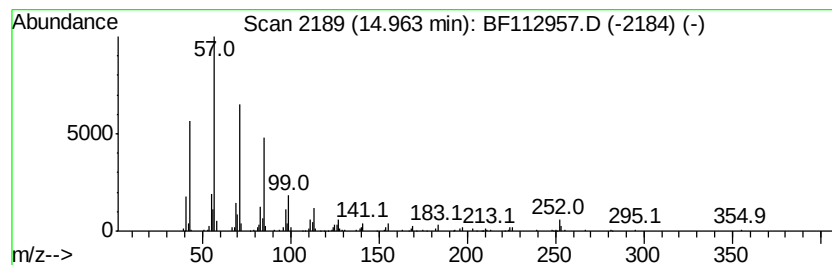
Instrument :
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ClientSampleId :
SD4-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.28 ng	280812	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Hexacosane	366 C26H54	000630-01-3	91
3	2-methyloctacosane	408 C29H60	1000376-72-8	91
4	triacontane	422 C30H62	000638-68-6	91
5	Eicosane	282 C20H42	000112-95-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112957.D
Acq On : 11 Mar 2019 16:25
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Sample : K1785-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

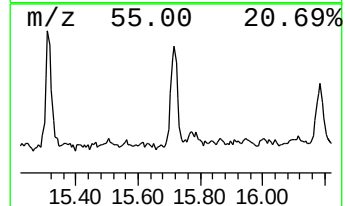
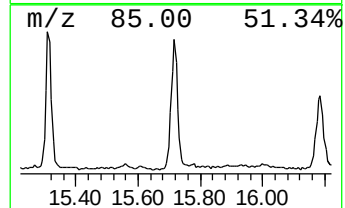
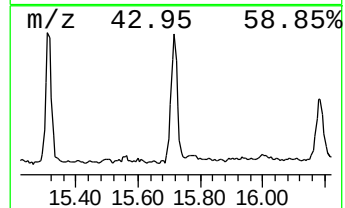
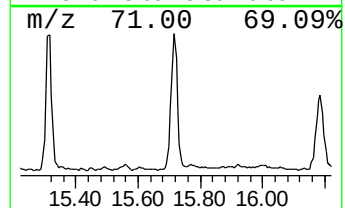
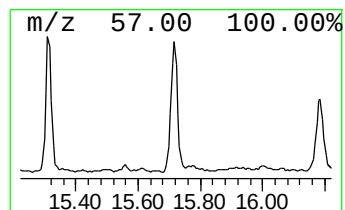
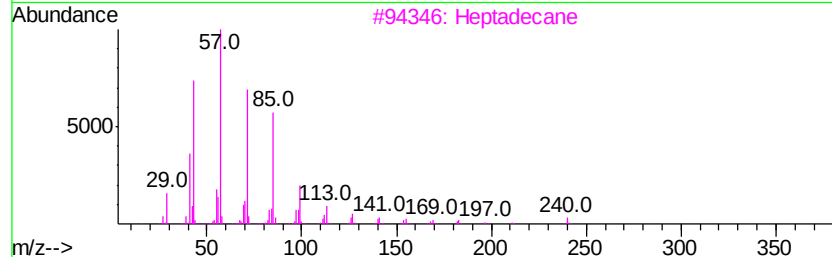
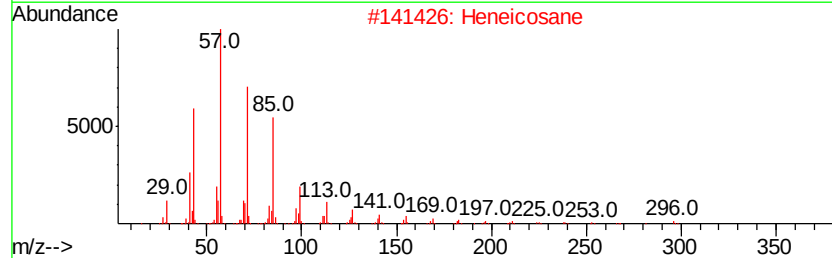
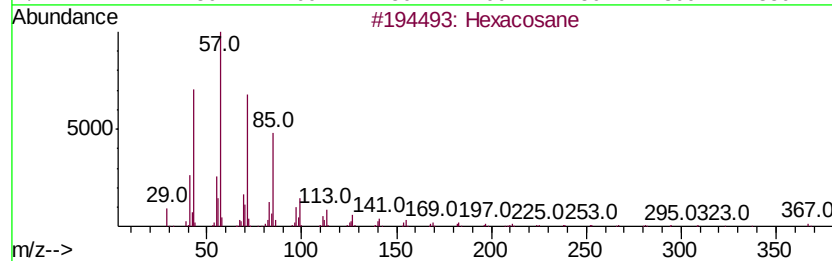
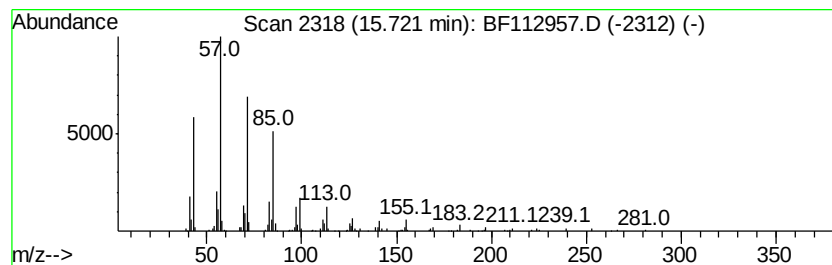
Instrument :
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ClientSampleId :
SD4-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	4.21 ng	360473	Perylene-d12	15.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	91
2	Heneicosane	296 C21H44	000629-94-7	91
3	Heptadecane	240 C17H36	000629-78-7	91
4	Octadecane	254 C18H38	000593-45-3	87
5	Octacosane	394 C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031119\
Data File : BF112957.D
Acq On : 11 Mar 2019 16:25
Operator : JU/SJ
Sample : K1785-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD4-0.0-0.5

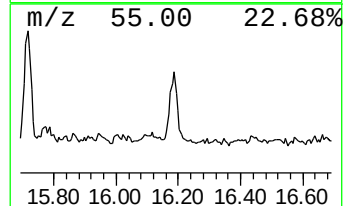
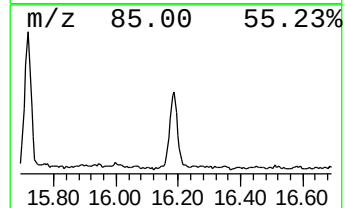
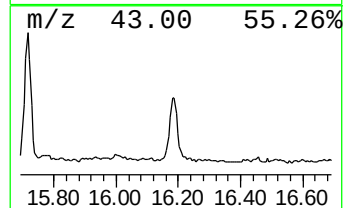
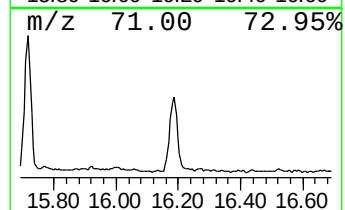
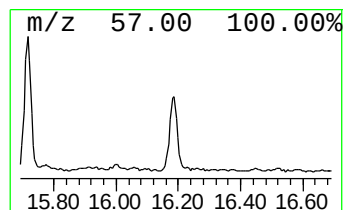
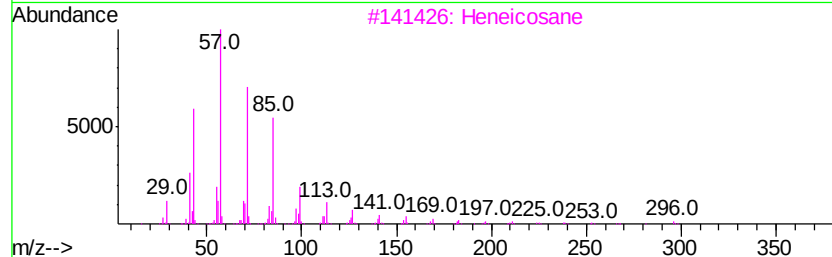
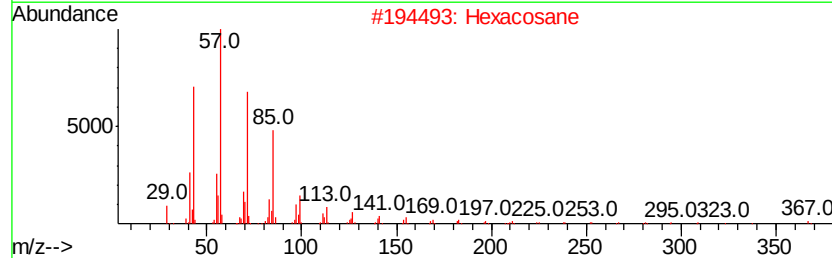
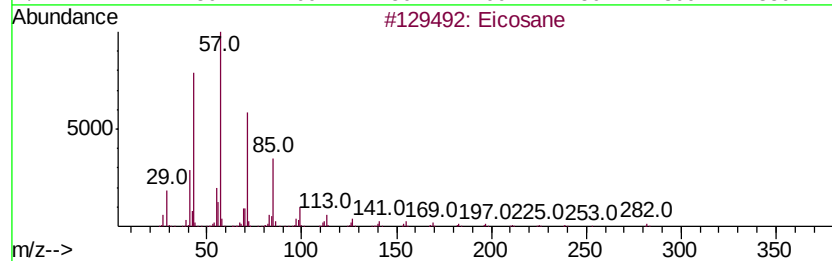
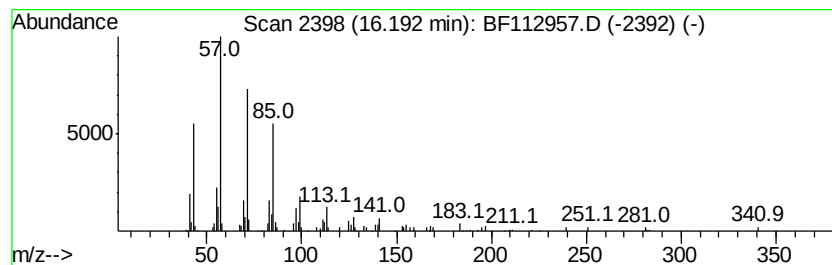
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.99 ng	255955	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
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		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031119\
Data File : BF112957.D
Acq On : 11 Mar 2019 16:25
Operator : JU/SJ
Sample : K1785-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SD4-0.0-0.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
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n-Hexadecanoic acid	11.77	8.7	ng	687135	4	11.24	1583580	20.0
unknown11.92	11.92	2.6	ng	204840	4	11.24	1583580	20.0
Octadecanoic acid	12.56	4.2	ng	433404	5	13.86	2070360	20.0
Heptadecyl heptaf...	13.73	2.3	ng	239369	5	13.86	2070360	20.0
Hexacosane	14.64	2.3	ng	199278	6	15.27	1712100	20.0
Heneicosane	14.96	3.3	ng	280812	6	15.27	1712100	20.0
Heptadecane	15.72	4.2	ng	360473	6	15.27	1712100	20.0
Eicosane	16.19	3.0	ng	255955	6	15.27	1712100	20.0