

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
 Data File : BF112614.D
 Acq On : 19 Feb 2019 12:01
 Operator : JU/SJ
 Sample : K1511-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STONES

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-BF012519.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	5.040	499	502	509	rBV	49347	70732	2.27%	0.265%
2	5.457	570	573	598	rBV	1445293	1657234	53.07%	6.212%
3	6.475	742	746	763	rBV	1557661	1756589	56.26%	6.584%
4	6.598	763	767	782	rVB	2093182	1915274	61.34%	7.179%
5	6.822	801	805	815	rBV	555302	501699	16.07%	1.880%
6	6.975	827	831	843	rBV	1576013	1517079	48.59%	5.686%
7	7.387	897	901	920	rBV	1094865	1144105	36.64%	4.288%
8	8.104	1019	1023	1046	rBV	675643	671953	21.52%	2.519%
9	9.175	1201	1205	1217	rBV	2634336	2472664	79.19%	9.268%
10	9.575	1269	1273	1278	rBV	77038	71908	2.30%	0.270%
11	9.857	1317	1321	1331	rBV	834598	809508	25.93%	3.034%
12	10.657	1453	1457	1466	rBV	1734735	1716253	54.96%	6.433%
13	11.351	1571	1575	1584	rBV	976318	912136	29.21%	3.419%
14	11.869	1659	1663	1678	rBV2	231002	304870	9.76%	1.143%
15	12.651	1792	1796	1807	rBV	135321	182333	5.84%	0.683%
16	12.933	1839	1844	1847	rBV	3229275	3122493	100.00%	11.704%
17	13.486	1933	1938	1941	rBV2	53519	61138	1.96%	0.229%
18	13.816	1990	1994	2004	rBV	175614	231806	7.42%	0.869%
19	13.998	2021	2025	2032	rBV	1032303	995625	31.89%	3.732%
20	14.127	2043	2047	2051	rBV	206169	191142	6.12%	0.716%
21	14.433	2094	2099	2103	rBV	492571	440777	14.12%	1.652%
22	14.733	2145	2150	2156	rBV	831042	860691	27.56%	3.226%
23	14.810	2159	2163	2169	rVB	195721	203384	6.51%	0.762%
24	15.068	2201	2207	2212	rBV	976780	1177101	37.70%	4.412%
25	15.439	2263	2270	2273	rBV	912532	1301883	41.69%	4.880%
26	15.468	2273	2275	2285	rVB	641691	793778	25.42%	2.975%
27	15.692	2310	2313	2319	rVB2	31585	44057	1.41%	0.165%
28	15.862	2335	2342	2351	rBV	616821	929938	29.78%	3.486%
29	16.357	2419	2426	2433	rBV	258432	465925	14.92%	1.746%
30	16.933	2518	2524	2531	rVB2	76514	155069	4.97%	0.581%

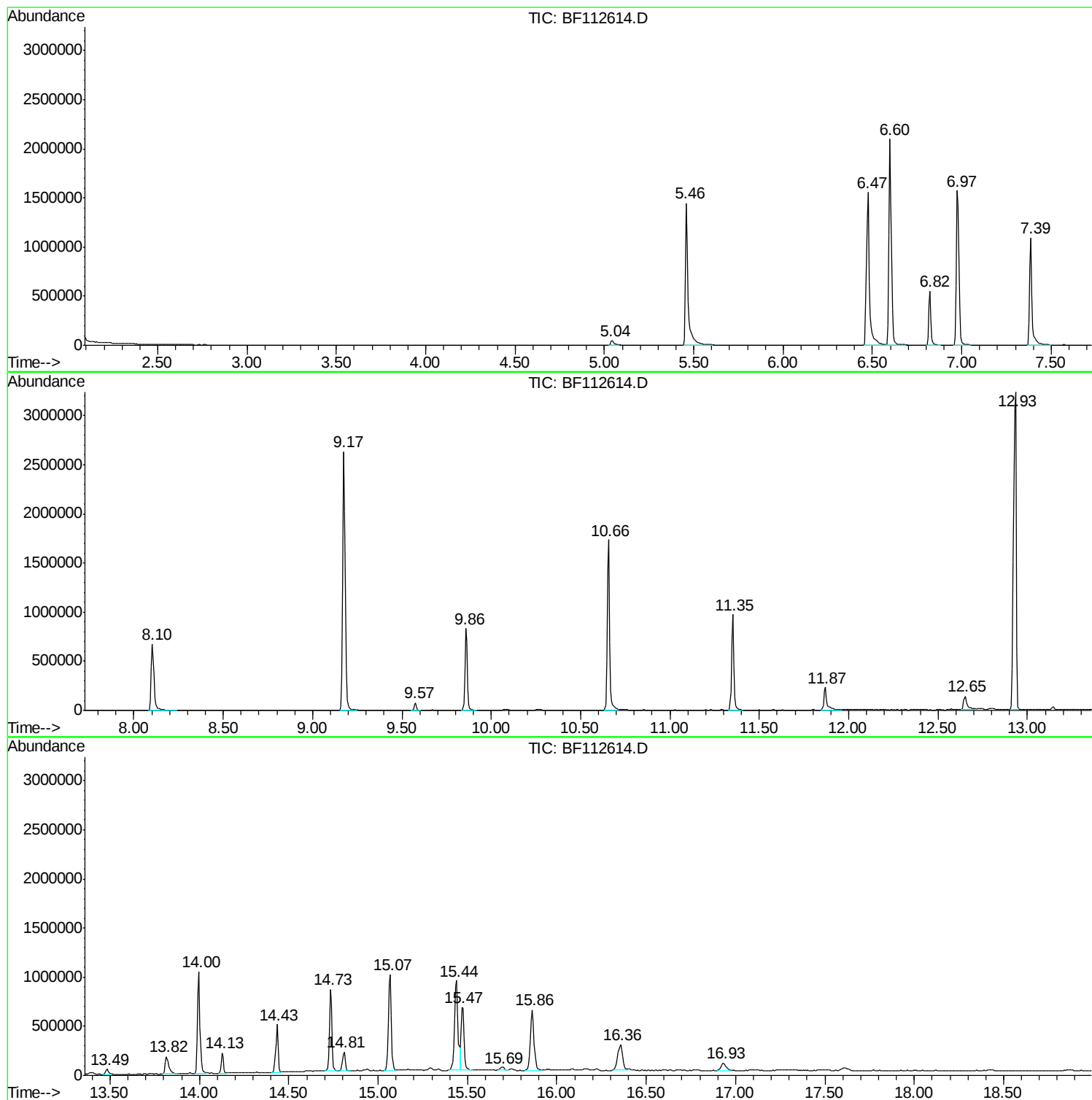
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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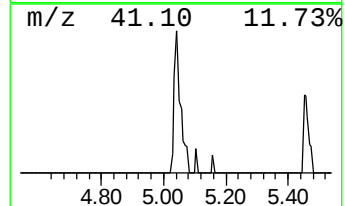
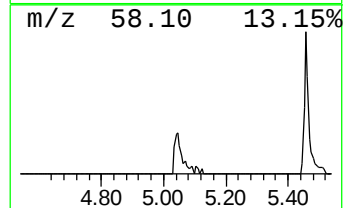
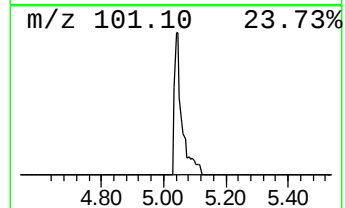
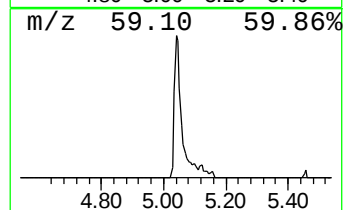
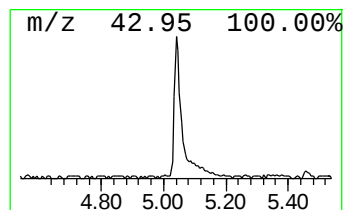
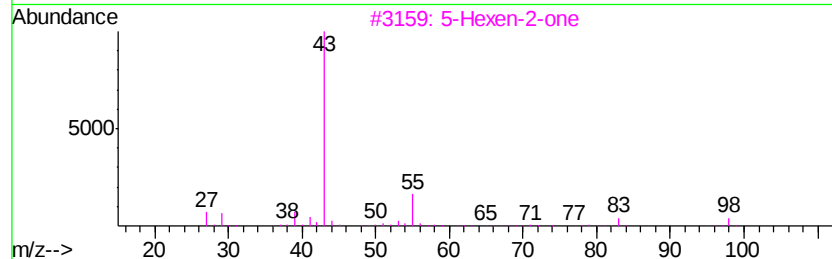
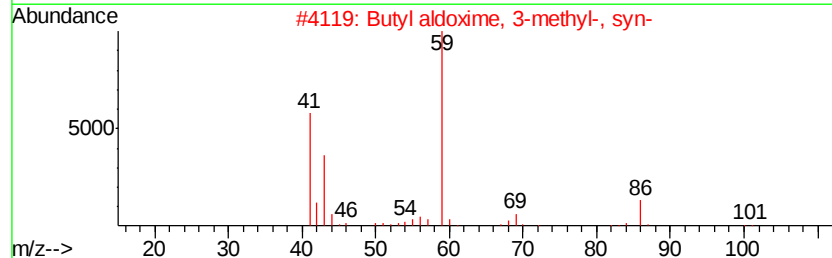
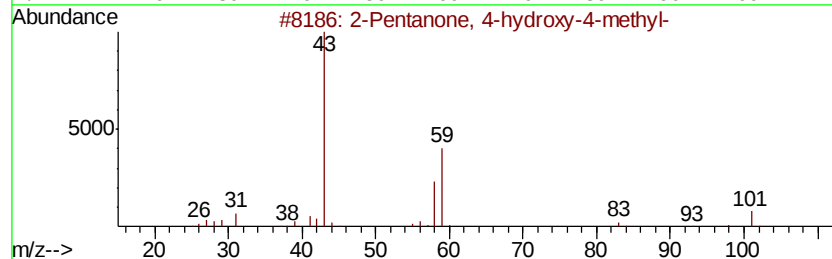
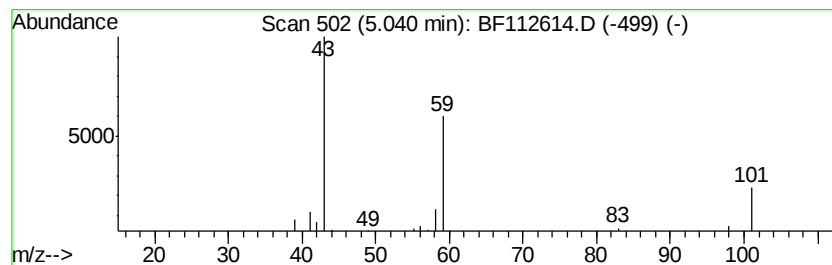
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	2.82 ng	70732	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9



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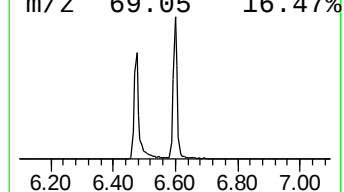
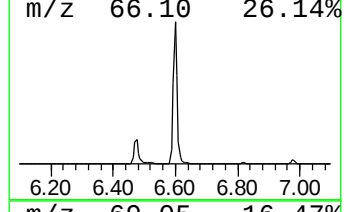
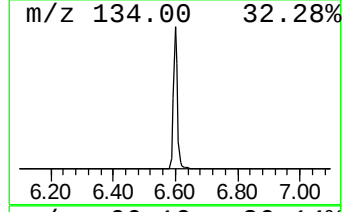
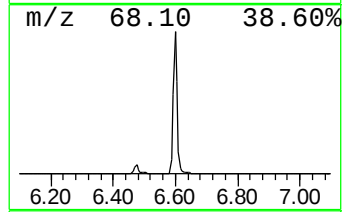
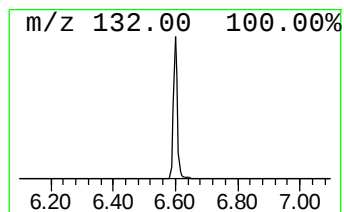
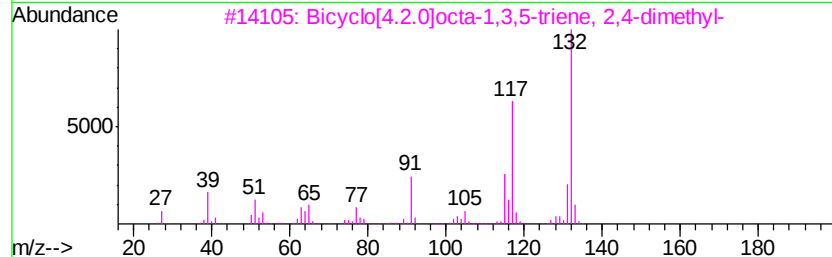
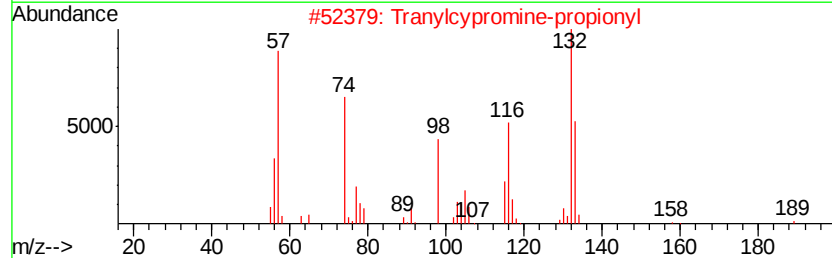
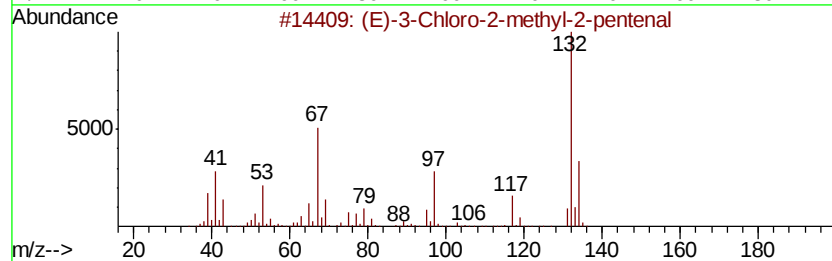
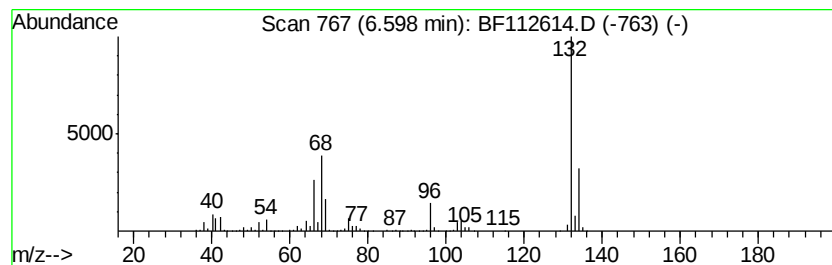
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	76.35 ng	1915270	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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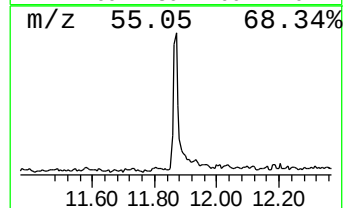
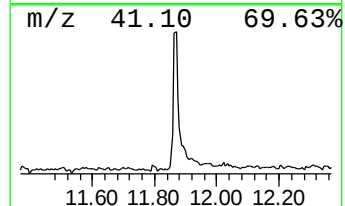
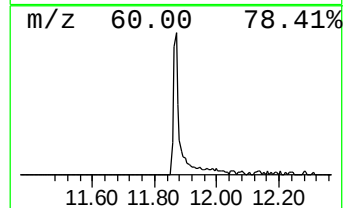
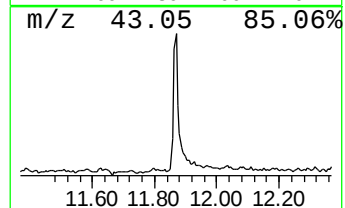
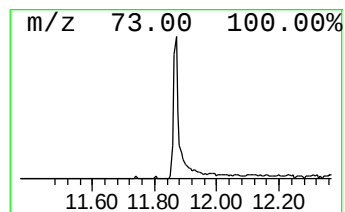
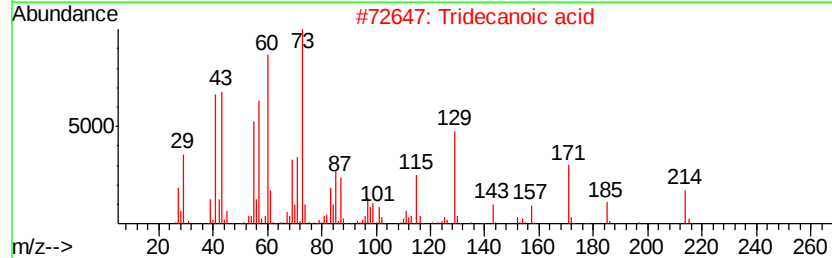
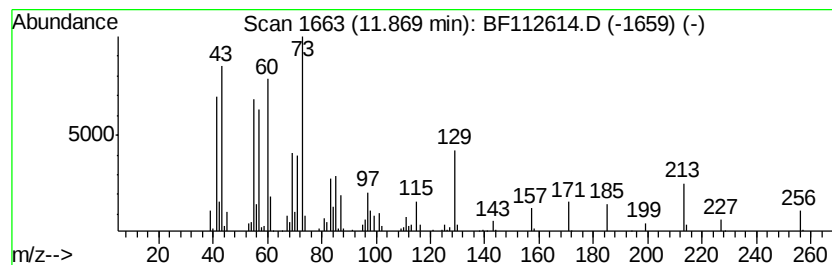
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	6.68 ng	304870	Phenanthrene-d10	11.35

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	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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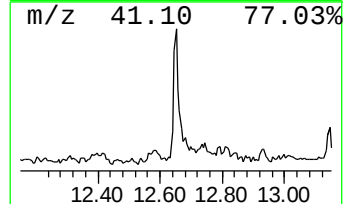
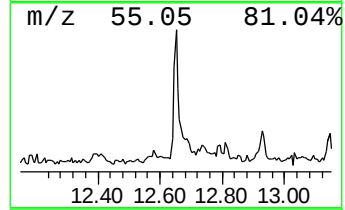
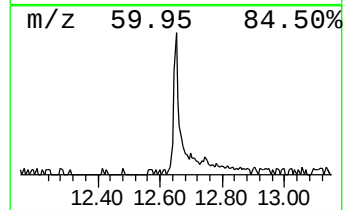
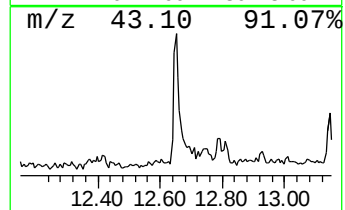
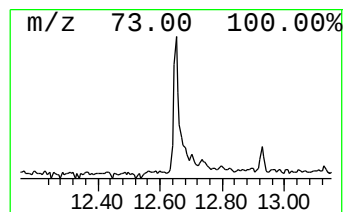
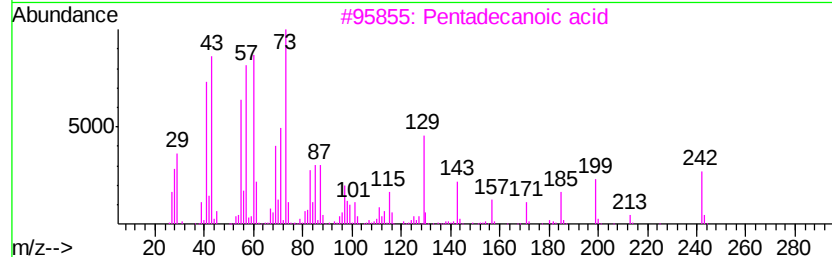
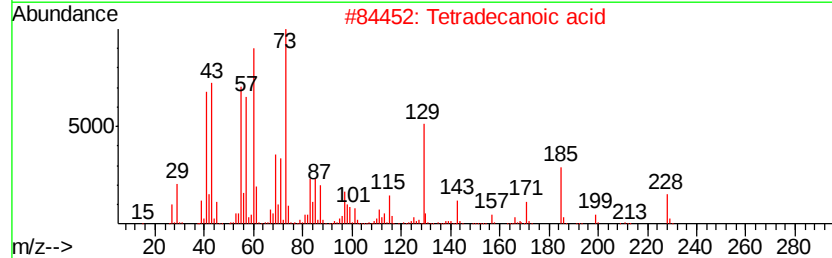
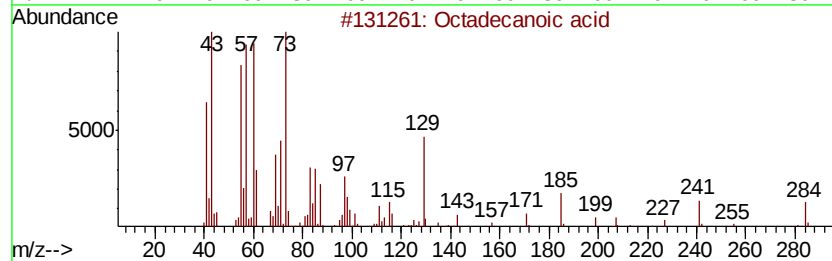
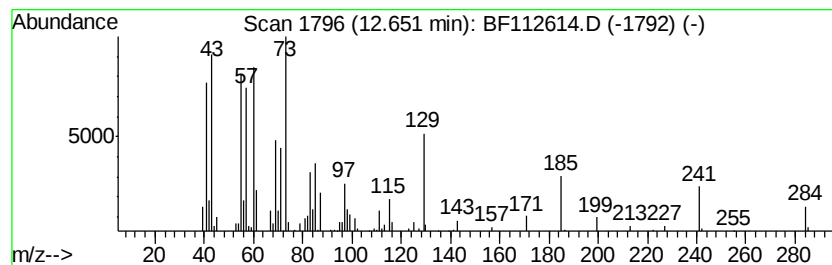
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.65	4.00 ng	182333	Phenanthrene-d10		11.35	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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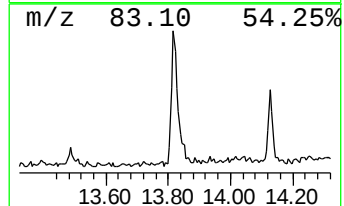
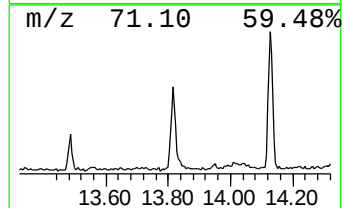
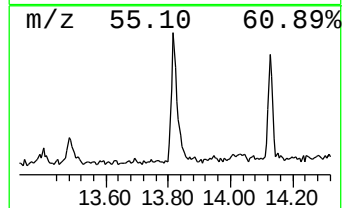
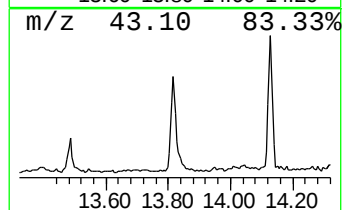
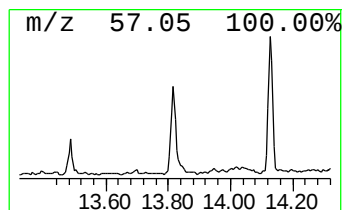
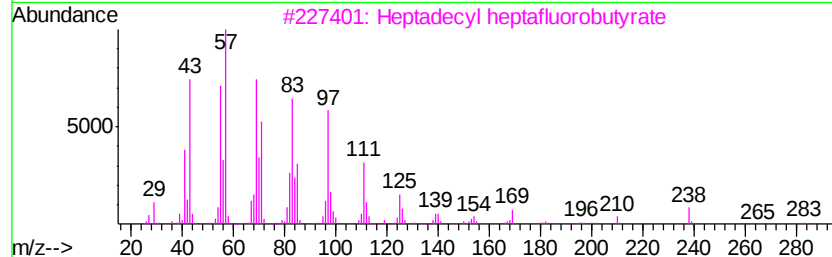
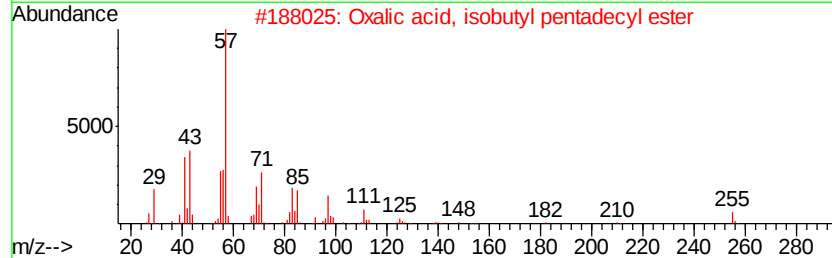
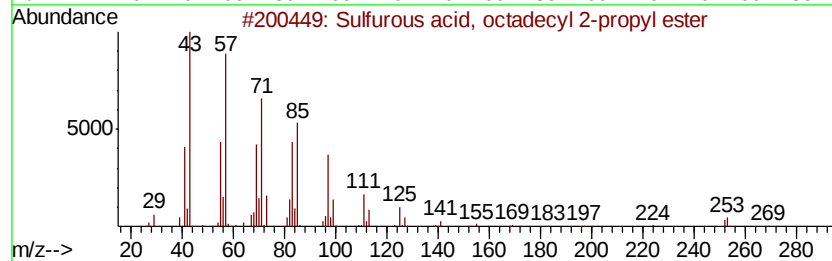
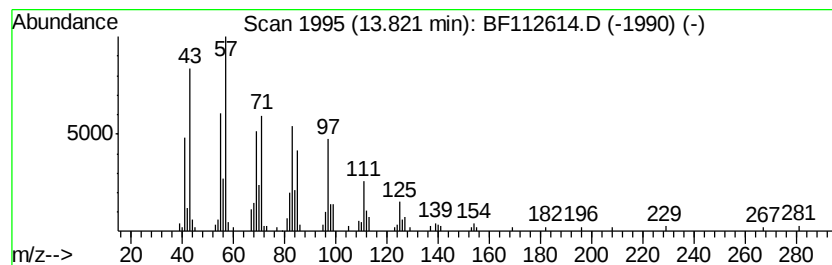
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 Peak Number 6 Sulfurous acid, octadecyl 2... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.66 ng	231806	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
2		Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
3		Heptadecyl heptafluorobutrate	452	C21H35F7O2	959085-66-6	64
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	64
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	62



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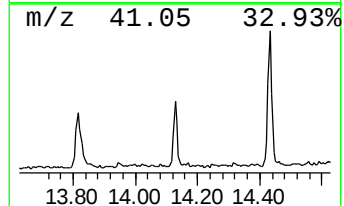
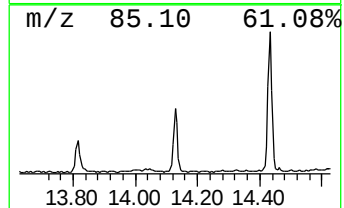
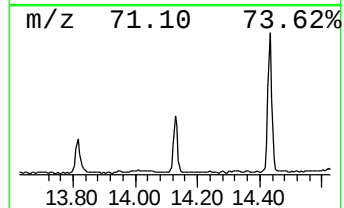
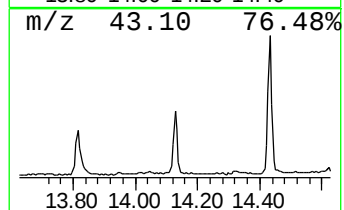
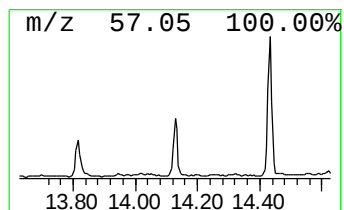
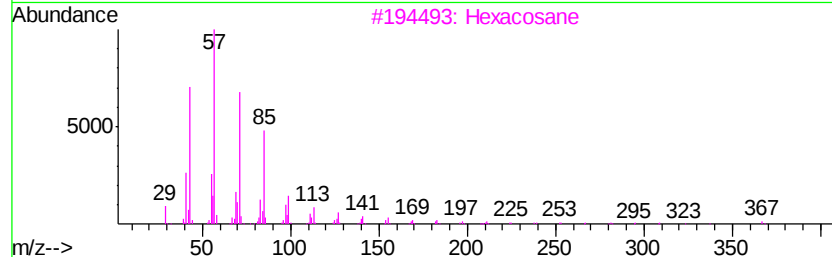
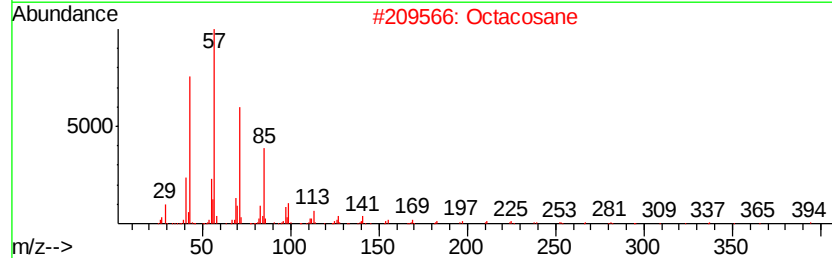
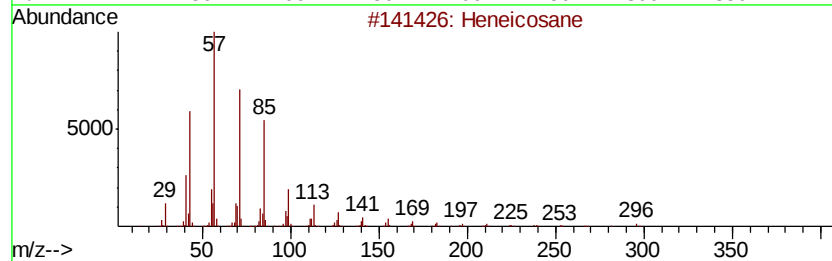
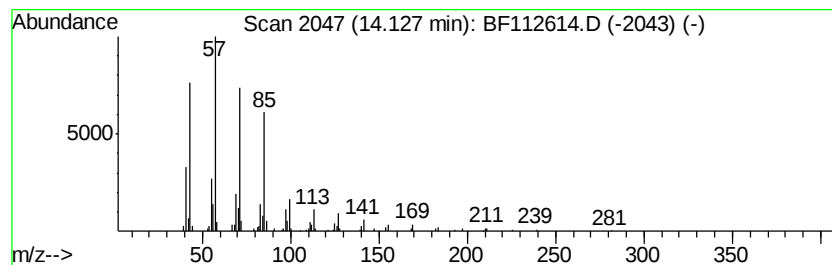
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane, 11-(1-ethylpro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	3.84 ng	191142	Chrysene-d12	14.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
Data File : BF112614.D
Acq On : 19 Feb 2019 12:01
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

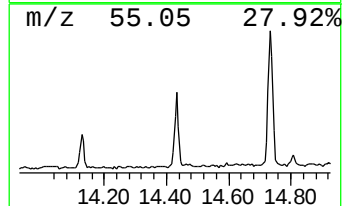
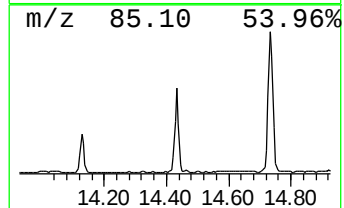
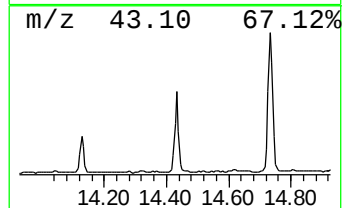
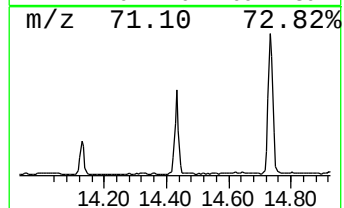
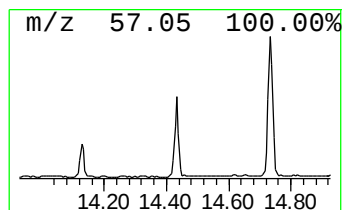
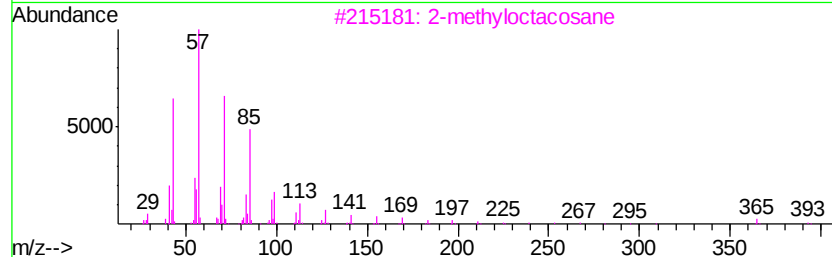
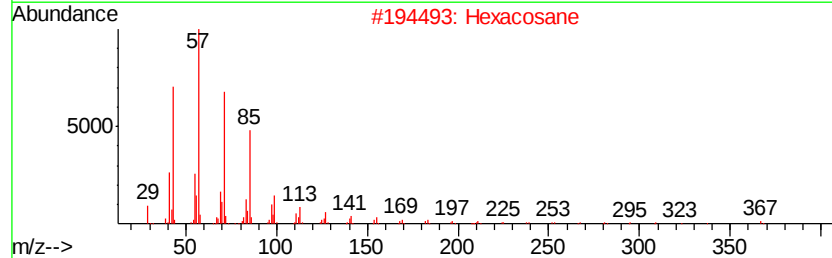
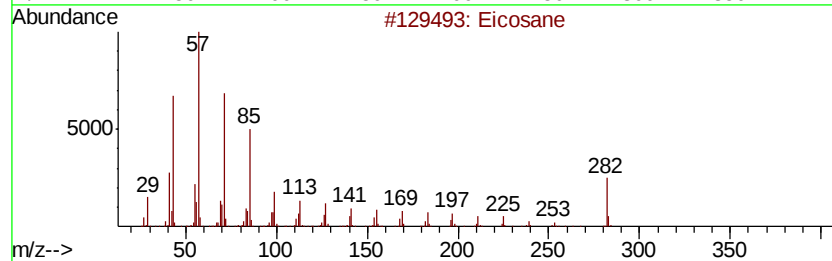
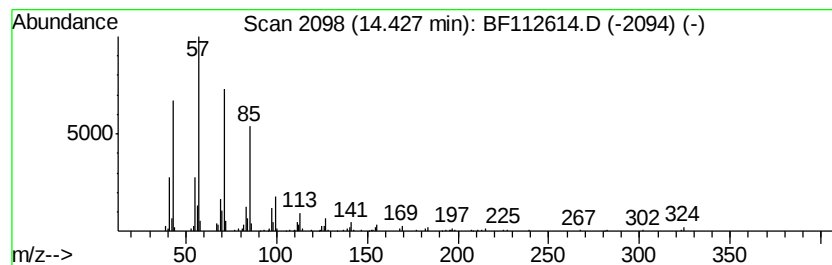
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ClientSampleId :
STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	8.85 ng	440777	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	93
2	Hexacosane	366 C26H54	000630-01-3	91
3	2-methyloctacosane	408 C29H60	1000376-72-8	91
4	Heneicosane	296 C21H44	000629-94-7	91
5	Octadecane	254 C18H38	000593-45-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
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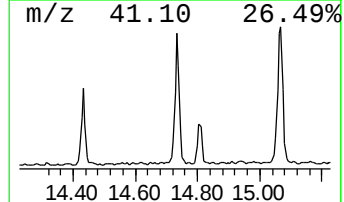
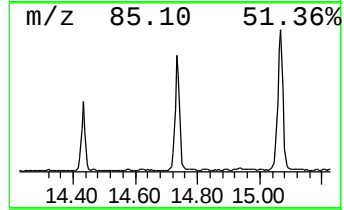
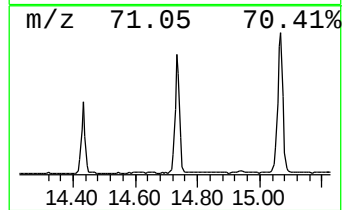
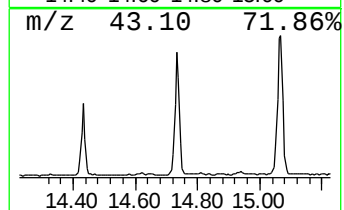
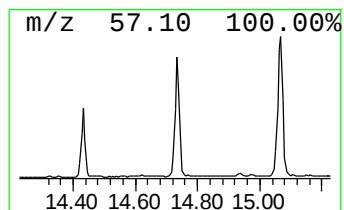
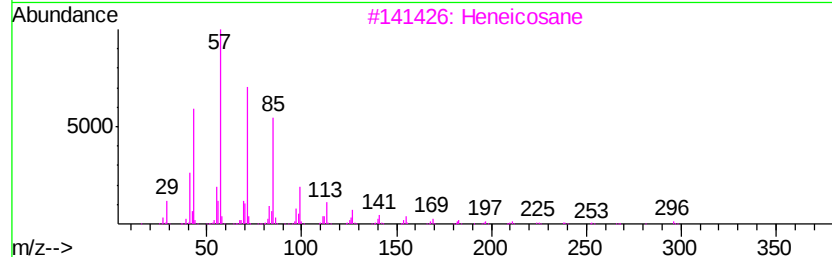
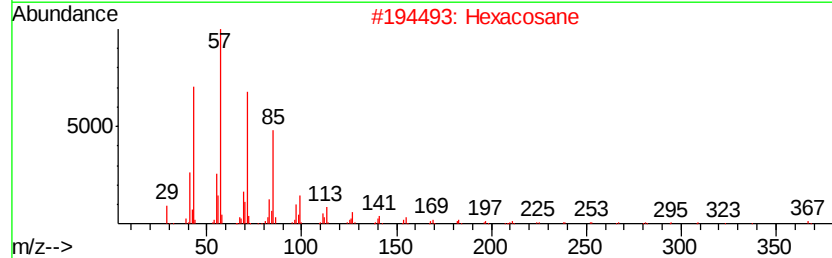
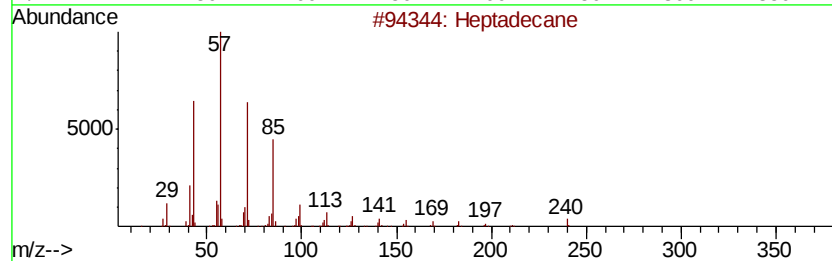
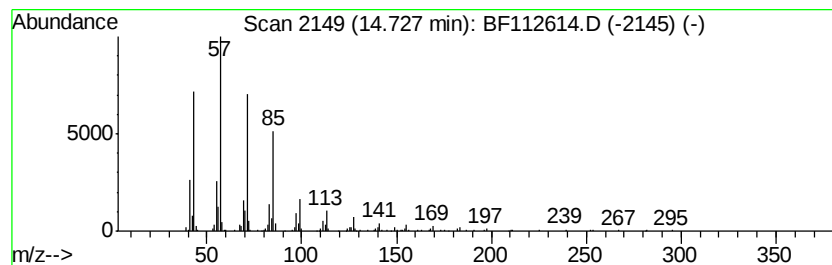
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	17.29 ng	860691	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	94
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heneicosane		296	C21H44	000629-94-7	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Tetracosane		338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
Data File : BF112614.D
Acq On : 19 Feb 2019 12:01
Operator : JU/SJ
Sample : K1511-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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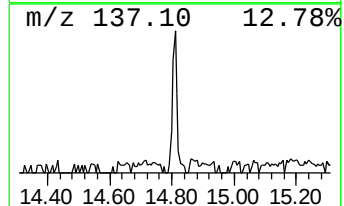
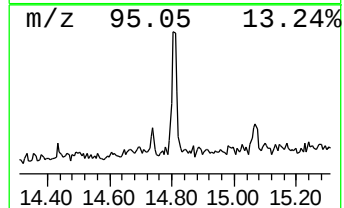
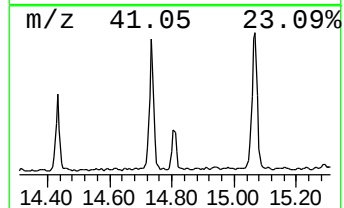
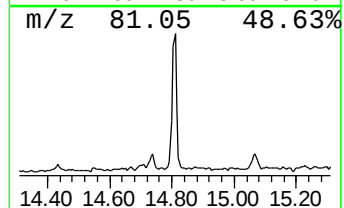
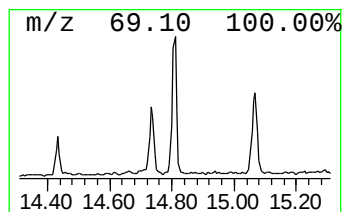
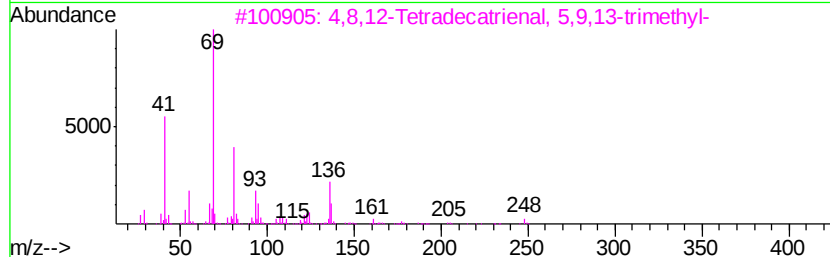
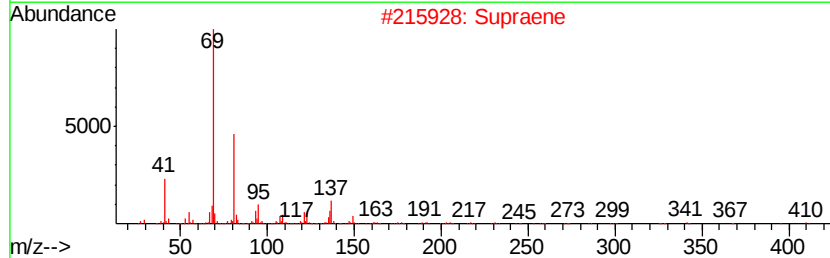
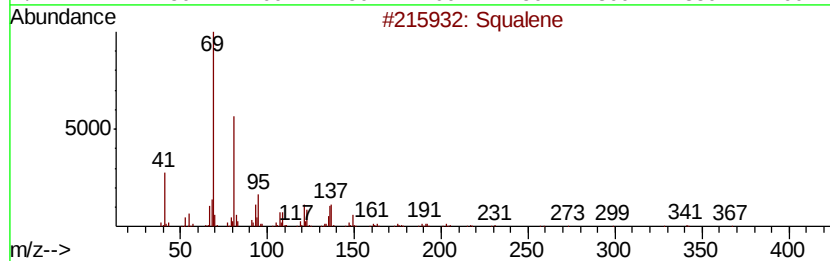
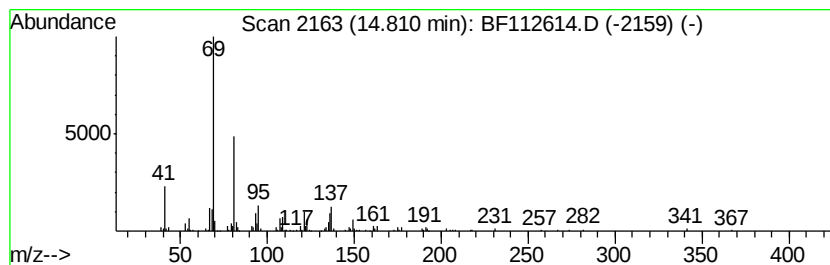
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	5.12 ng	203384	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
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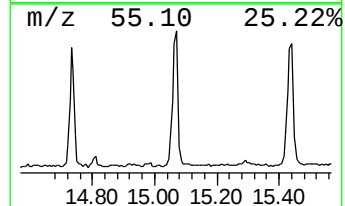
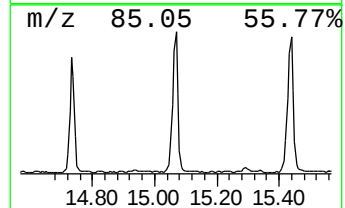
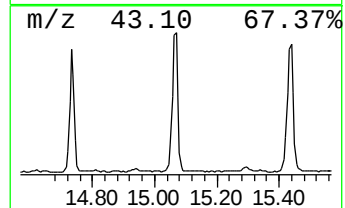
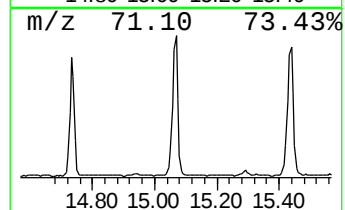
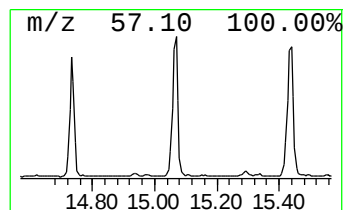
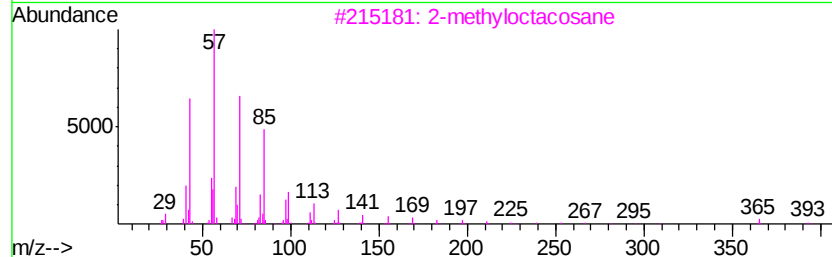
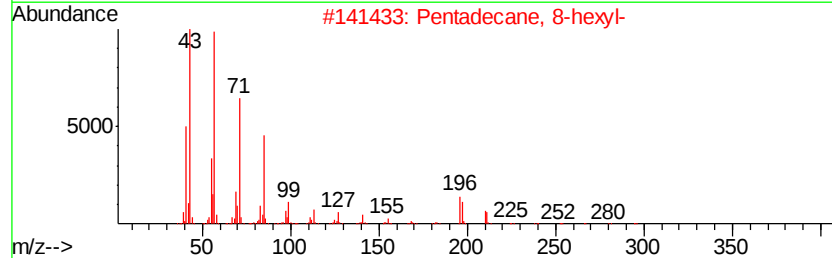
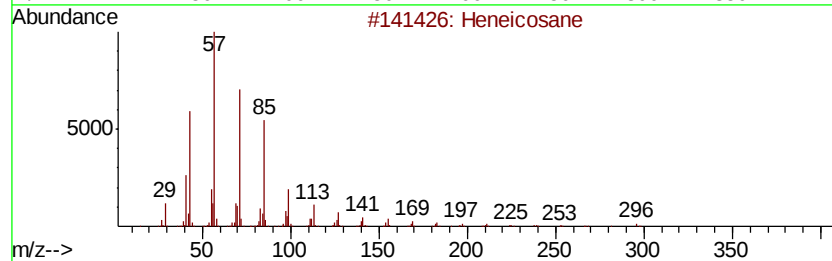
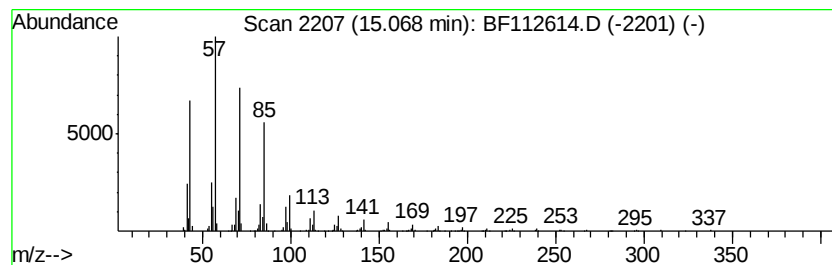
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	29.66 ng	1177100	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	96
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
Data File : BF112614.D
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ClientSampleId :
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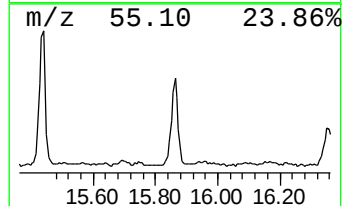
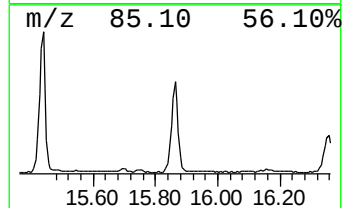
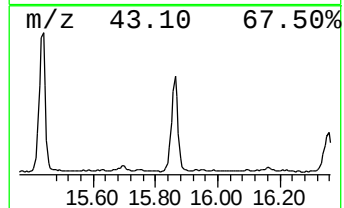
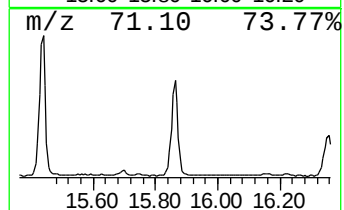
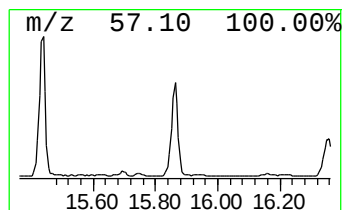
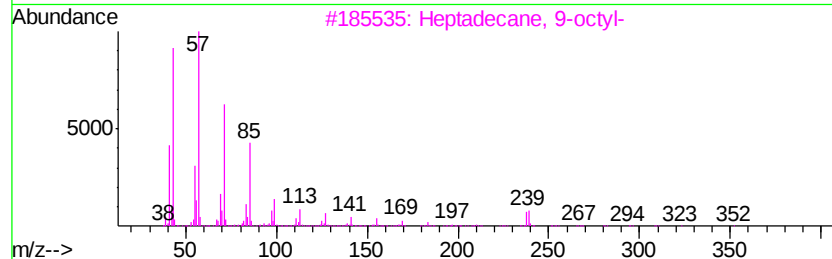
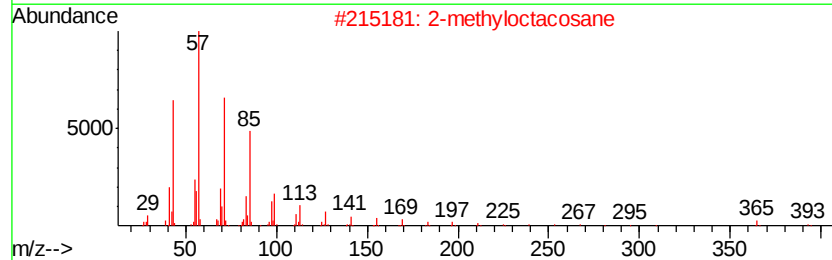
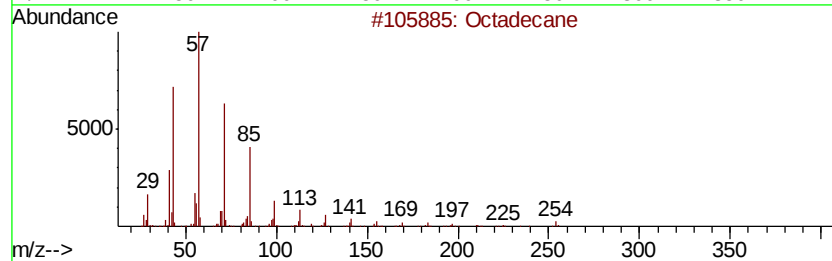
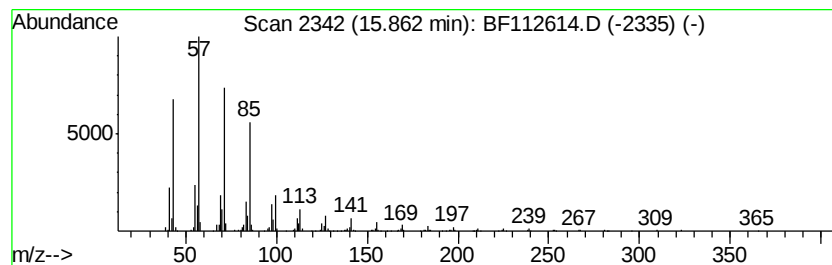
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	23.43 ng	929938	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	94
2		2-methyloctacosane	408	C29H60	1000376-72-8	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
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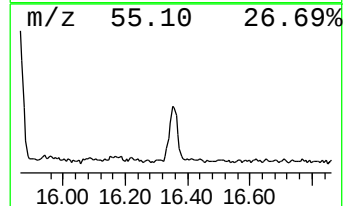
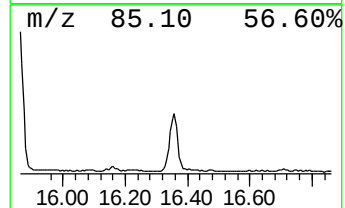
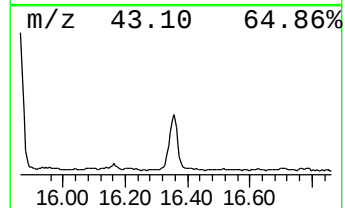
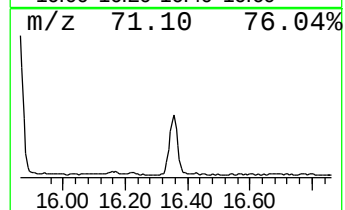
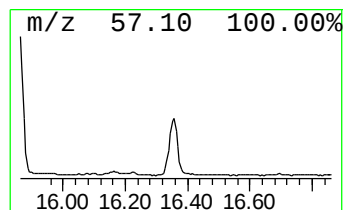
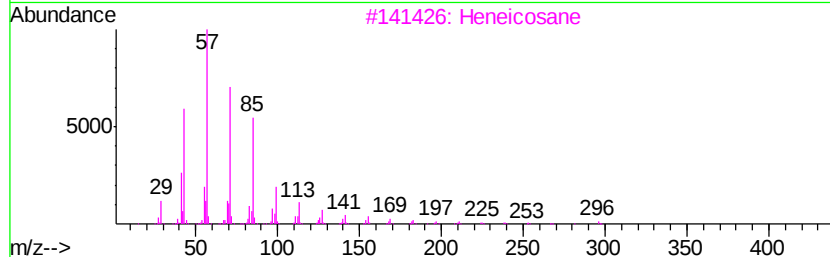
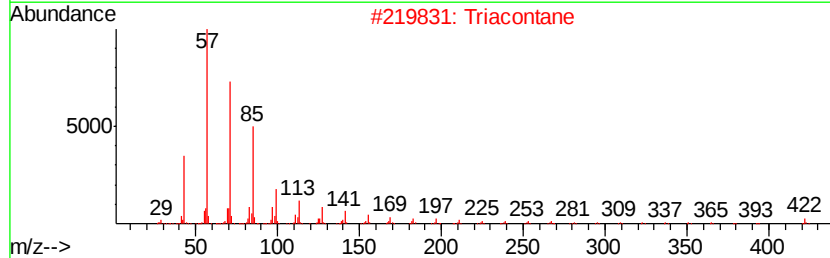
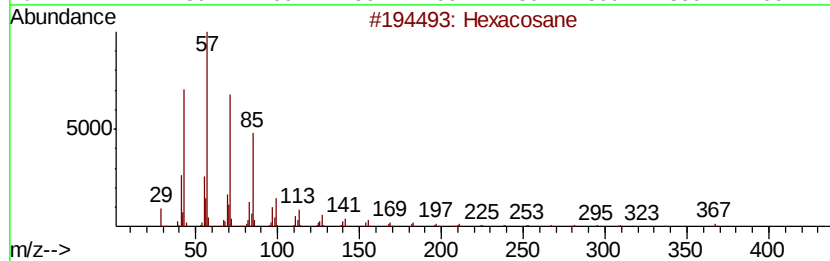
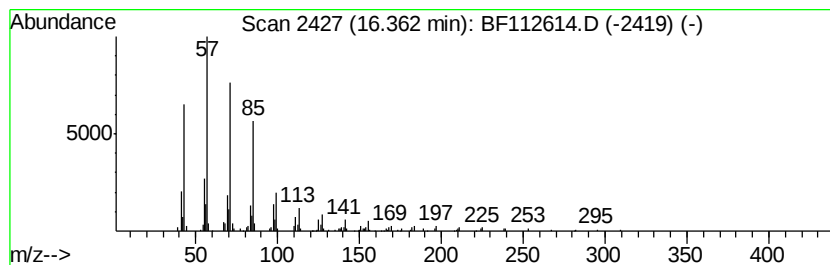
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	11.74 ng	465925	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Triacontane	422	C30H62	000638-68-6	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Docosane	310	C22H46	000629-97-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
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ClientSampleId :
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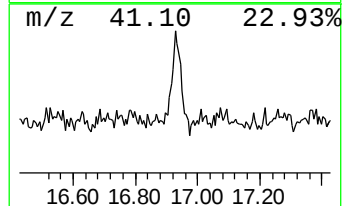
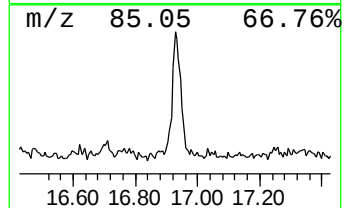
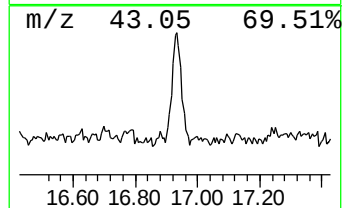
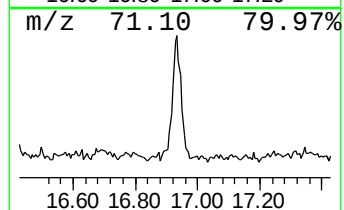
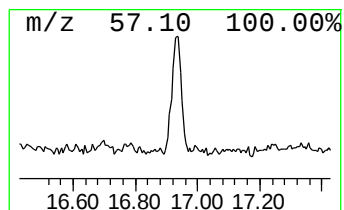
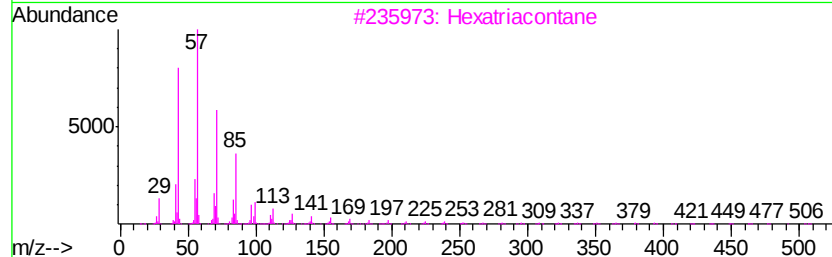
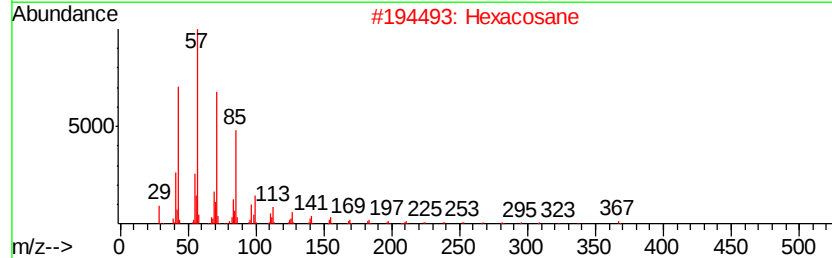
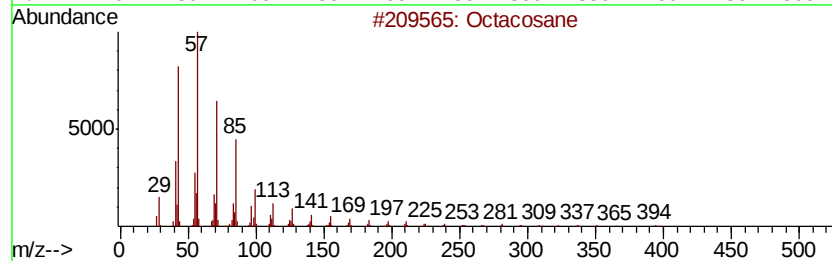
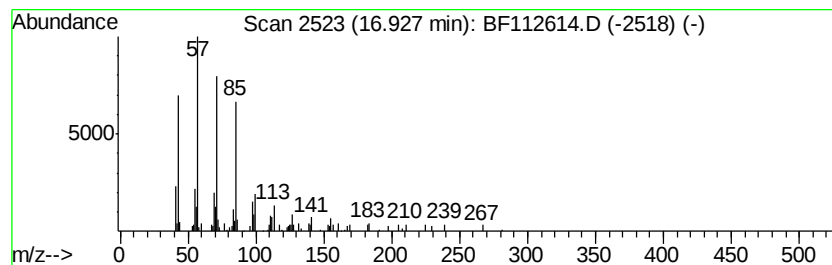
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.93	3.91 ng	155069	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Hexatriacontane	507	C36H74	000630-06-8	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021919\
 Data File : BF112614.D
 Acq On : 19 Feb 2019 12:01
 Operator : JU/SJ
 Sample : K1511-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 STONES

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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
2-Pentanone, 4-hy...	5.04	2.8	ng	70732	1	6.82	501699	20.0
unknown6.60	6.60	76.3	ng	1915270	1	6.82	501699	20.0
n-Hexadecanoic acid	11.87	6.7	ng	304870	4	11.35	912136	20.0
Octadecanoic acid	12.65	4.0	ng	182333	4	11.35	912136	20.0
Sulfurous acid, o...	13.82	4.7	ng	231806	5	14.00	995625	20.0
Heneicosane, 11-(...	14.13	3.8	ng	191142	5	14.00	995625	20.0
Eicosane	14.43	8.8	ng	440777	5	14.00	995625	20.0
Heptadecane	14.73	17.3	ng	860691	5	14.00	995625	20.0
Squalene	14.81	5.1	ng	203384	6	15.47	793778	20.0
Heneicosane	15.07	29.7	ng	1177100	6	15.47	793778	20.0
Octadecane	15.86	23.4	ng	929938	6	15.47	793778	20.0
Hexacosane	16.36	11.7	ng	465925	6	15.47	793778	20.0
Octacosane	16.93	3.9	ng	155069	6	15.47	793778	20.0