

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
 Data File : BF112277.D
 Acq On : 28 Jan 2019 16:25
 Operator : JU/SJ
 Sample : K1261-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-C05

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	2.163	5	13	18	rVB	182080	242535	3.16%	0.369%
2	5.081	505	509	521	rVB	203437	319047	4.16%	0.486%
3	5.487	573	578	581	rBV	5460674	5610576	73.21%	8.543%
4	6.492	743	749	752	rBV	5246543	6071525	79.23%	9.245%
5	6.622	766	771	774	rBV	6470435	6282630	81.98%	9.567%
6	6.839	805	808	816	rBV	1570159	1320524	17.23%	2.011%
7	6.998	831	835	839	rBV	5248551	4973151	64.90%	7.573%
8	7.404	898	904	907	rBV	3607707	3917786	51.12%	5.966%
9	8.122	1020	1026	1033	rBV	1915929	1801249	23.51%	2.743%
10	8.545	1094	1098	1100	rBV	77389	81387	1.06%	0.124%
11	9.198	1203	1209	1212	rBV	7557191	7449495	97.21%	11.343%
12	9.586	1272	1275	1279	rBV	497028	461704	6.02%	0.703%
13	9.875	1317	1324	1328	rBV	2161262	2084704	27.20%	3.174%
14	10.669	1454	1459	1472	rBV	4648996	5266478	68.72%	8.019%
15	11.363	1573	1577	1580	rBV	2536731	2247888	29.33%	3.423%
16	11.386	1580	1581	1585	rVB	259373	152157	1.99%	0.232%
17	11.892	1664	1667	1673	rVB3	570032	575899	7.52%	0.877%
18	11.974	1678	1681	1684	rBV2	72791	85086	1.11%	0.130%
19	12.404	1750	1754	1758	rBV2	86513	126435	1.65%	0.193%
20	12.574	1780	1783	1789	rBV	564106	492716	6.43%	0.750%
21	12.669	1796	1799	1806	rBV2	101369	101186	1.32%	0.154%
22	12.804	1816	1822	1826	rBV	488585	516032	6.73%	0.786%
23	12.951	1841	1847	1850	rBV	7493571	7663241	100.00%	11.669%
24	13.239	1892	1896	1900	rBV2	54521	85436	1.11%	0.130%
25	13.510	1939	1942	1944	rBV	91007	82575	1.08%	0.126%
26	13.827	1993	1996	2007	rVB2	759841	1035138	13.51%	1.576%
27	14.004	2021	2026	2029	rBV	2130109	2121790	27.69%	3.231%
28	14.027	2029	2030	2036	rVB	194140	134136	1.75%	0.204%
29	14.151	2048	2051	2057	rBV	159225	172410	2.25%	0.263%
30	14.457	2100	2103	2111	rVB	274666	339734	4.43%	0.517%
31	14.757	2151	2154	2159	rVB	255286	267870	3.50%	0.408%
32	14.833	2164	2167	2172	rVB	285683	291690	3.81%	0.444%
33	15.039	2199	2202	2205	rBV	148343	208555	2.72%	0.318%
34	15.092	2208	2211	2219	rVB	347576	427711	5.58%	0.651%

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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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35	15.339	2251	2253	2260	rVB	107800	163790	2.14%	0.249%
36	15.404	2261	2264	2269	rBV	103140	126895	1.66%	0.193%
37	15.468	2270	2275	2283	rBV	1382174	1785523	23.30%	2.719%
38	15.898	2343	2348	2353	rBV	257104	399344	5.21%	0.608%
39	16.398	2429	2433	2437	rBV2	117277	186531	2.43%	0.284%

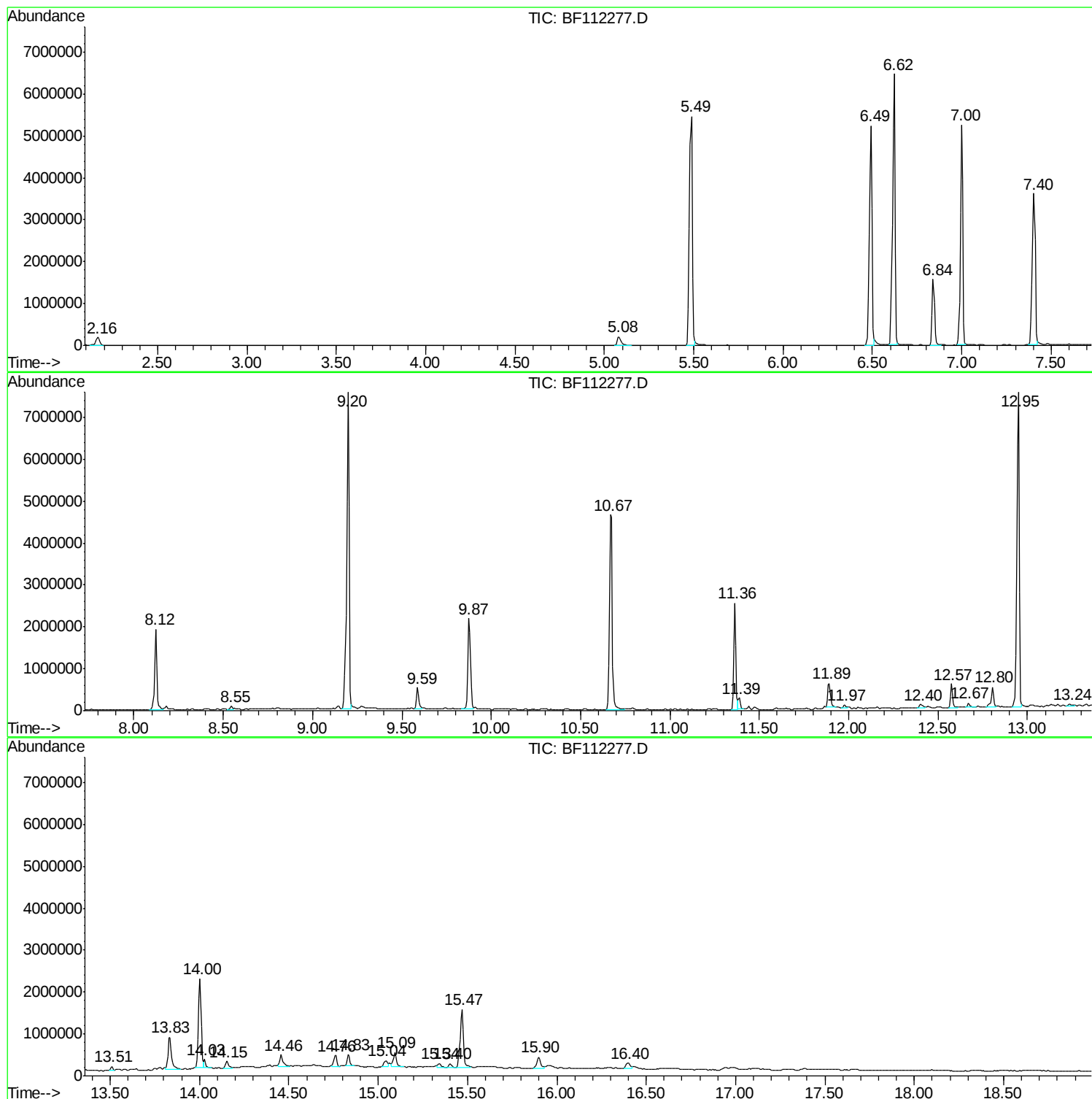
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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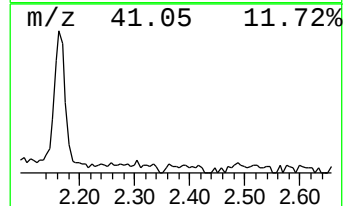
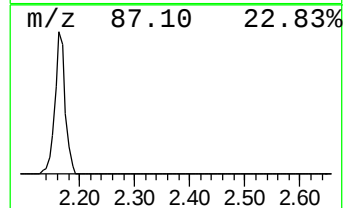
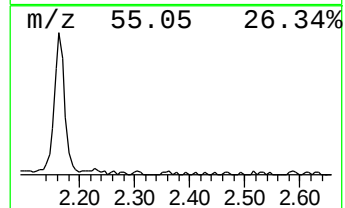
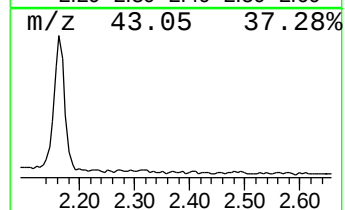
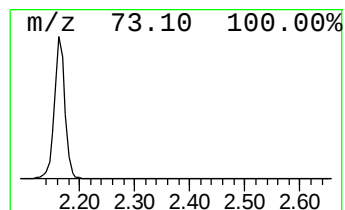
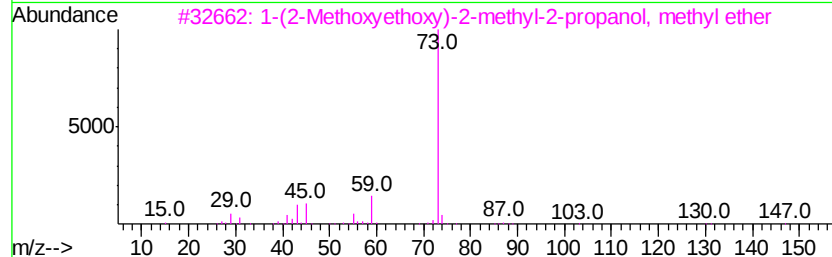
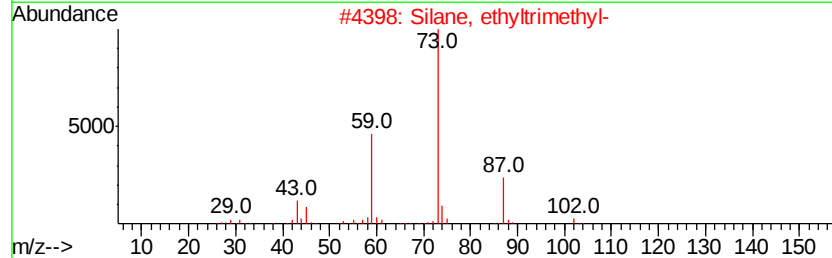
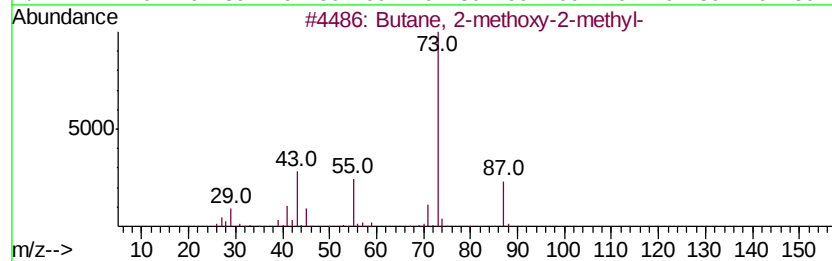
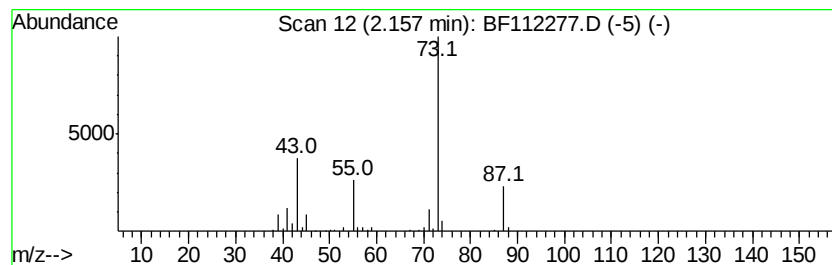
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	3.67 ng	242535	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	36
3		1-(2-Methoxyethoxy)-2-methyl-2-propanol, methyl ether	162	C8H18O3	1000364-24-4	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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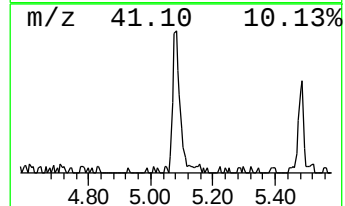
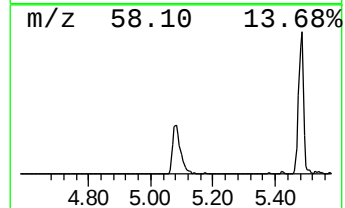
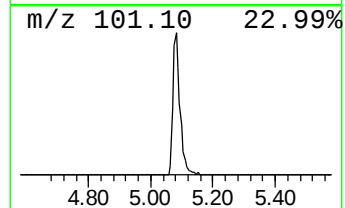
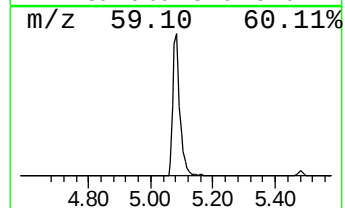
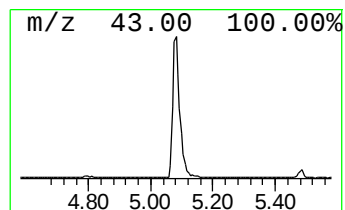
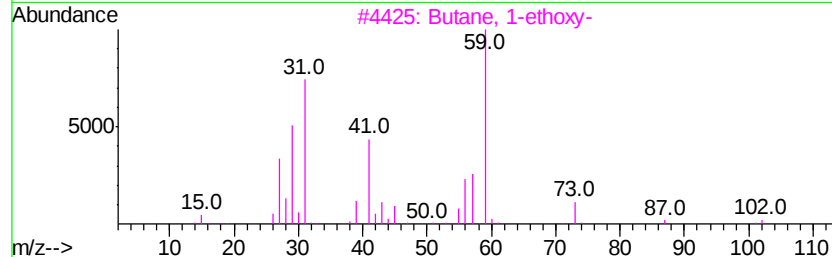
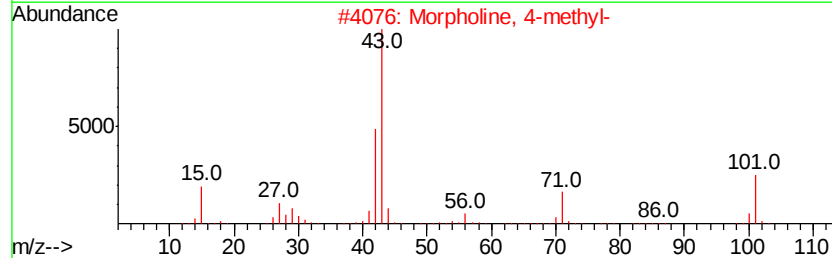
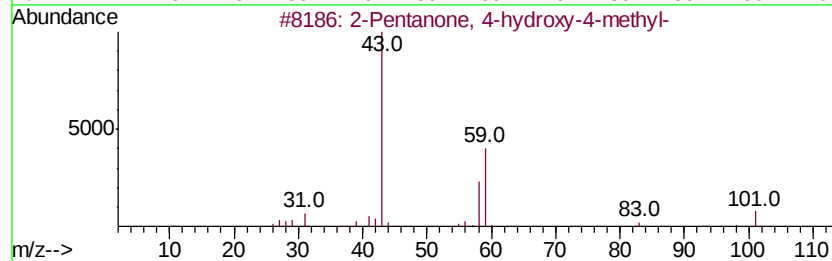
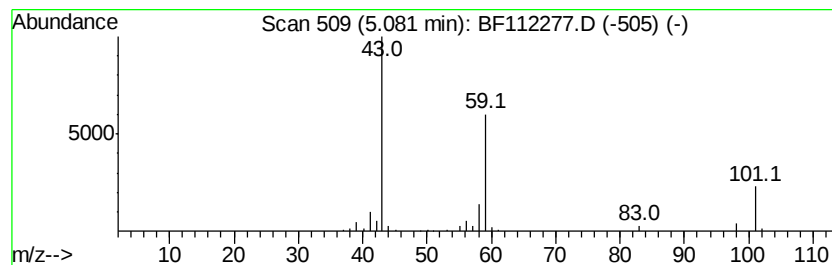
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	4.83 ng	319047	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane	58	C4H10	000106-97-8	9



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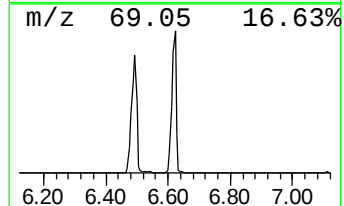
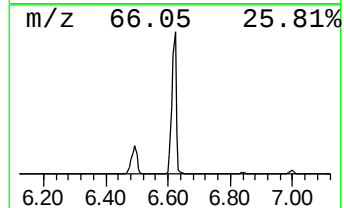
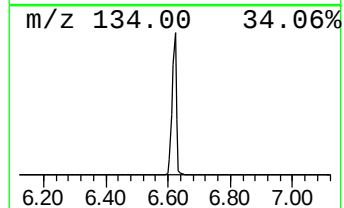
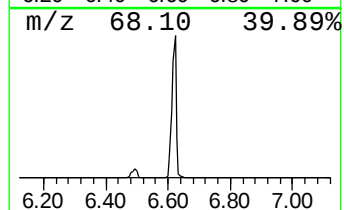
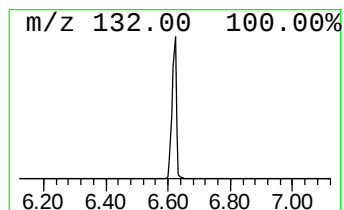
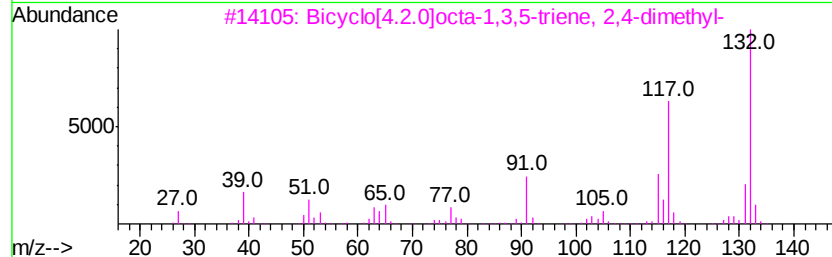
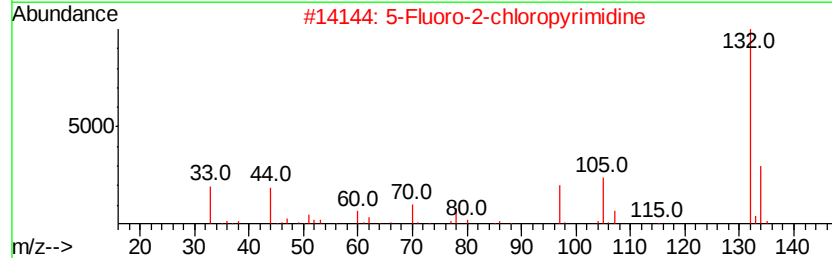
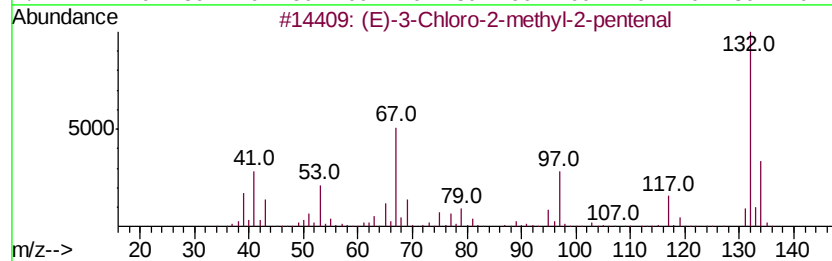
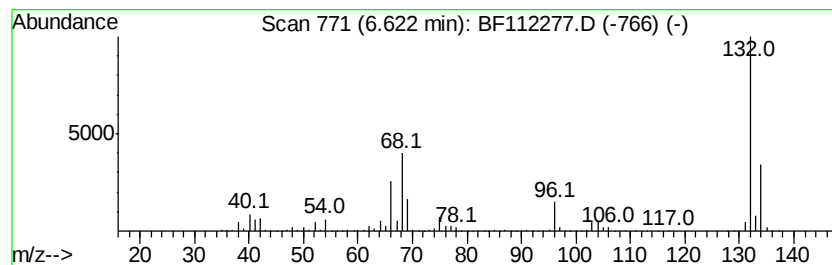
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	95.15 ng	6282630	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Xenon	132	Xe	007440-63-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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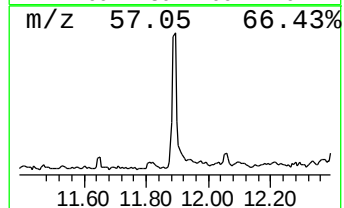
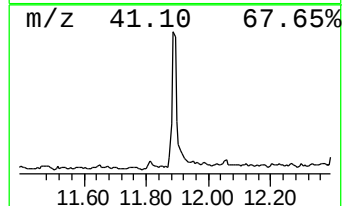
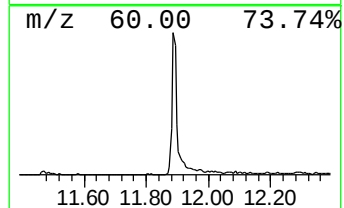
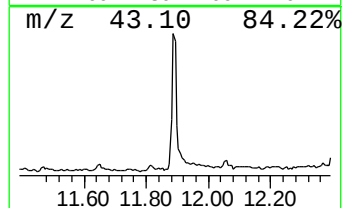
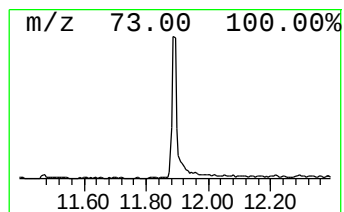
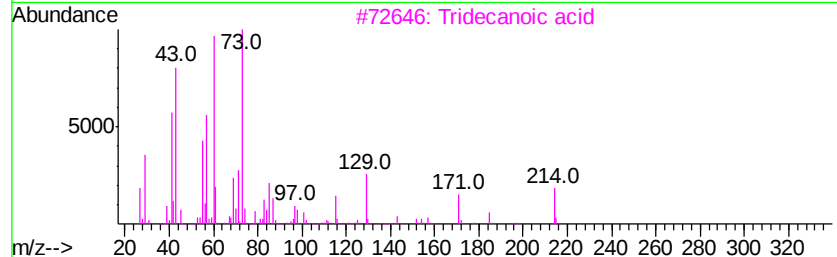
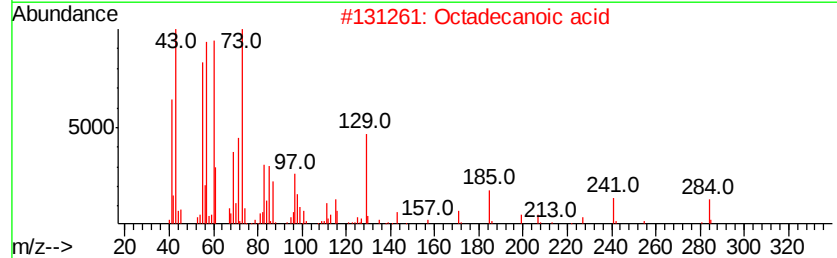
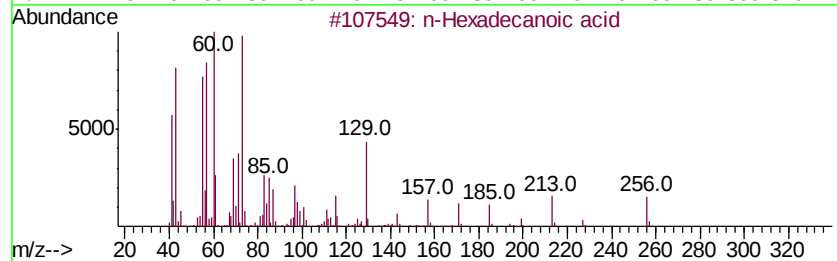
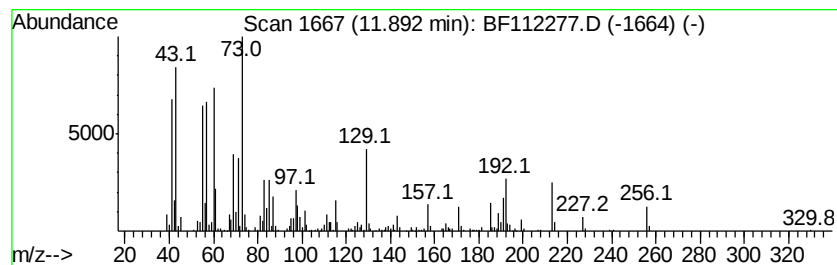
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	5.12 ng	575899	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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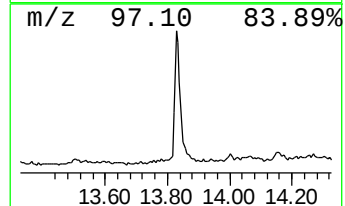
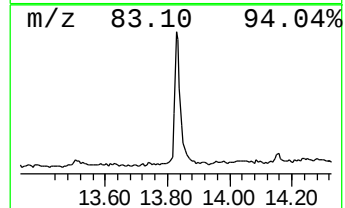
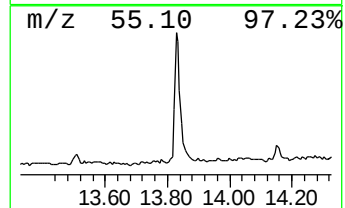
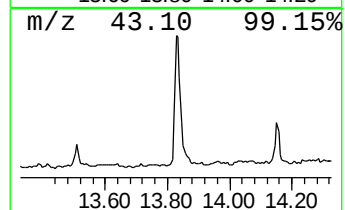
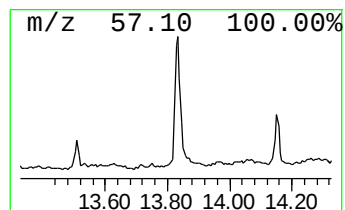
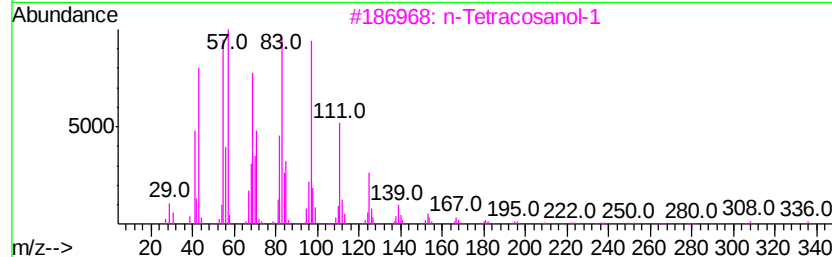
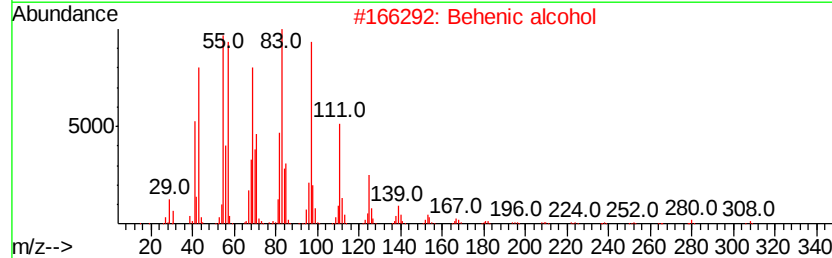
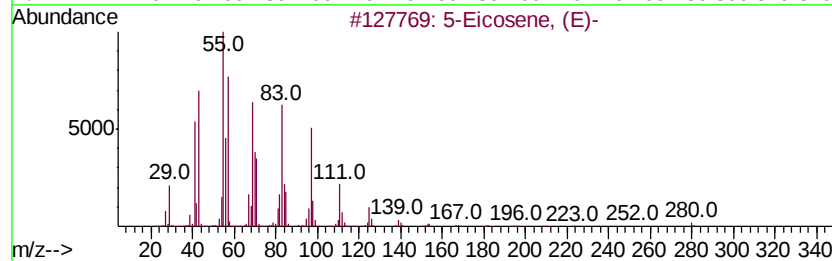
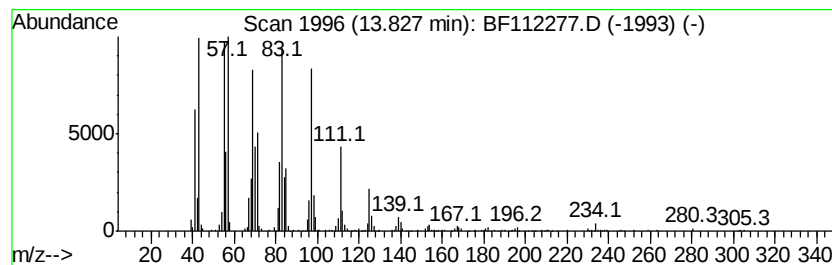
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	9.76 ng	1035140	Chrysene-d12	14.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
Data File : BF112277.D
Acq On : 28 Jan 2019 16:25
Operator : JU/SJ
Sample : K1261-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

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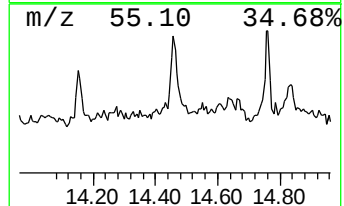
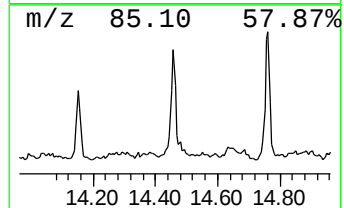
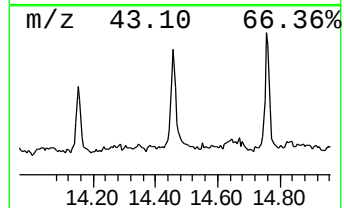
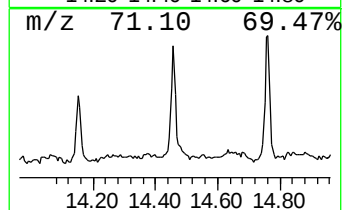
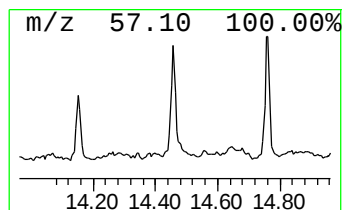
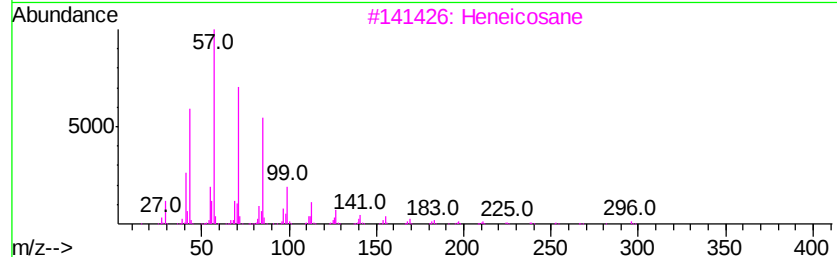
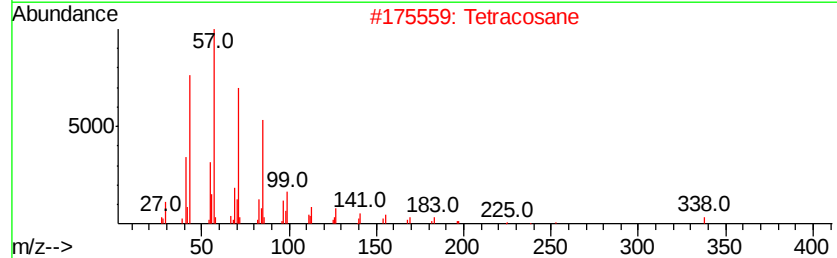
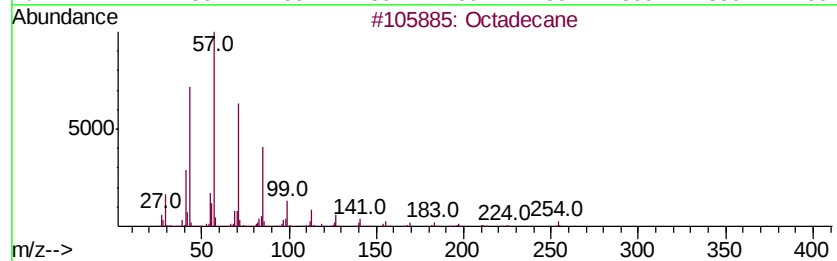
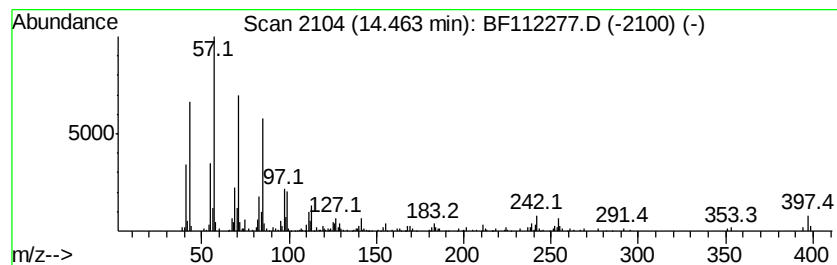
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	3.20 ng	339734	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	91
2		Tetracosane	338	C24H50	000646-31-1	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	90
5		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
Data File : BF112277.D
Acq On : 28 Jan 2019 16:25
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Sample : K1261-03
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ClientSampleId :
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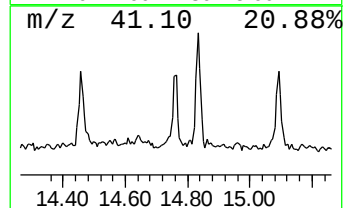
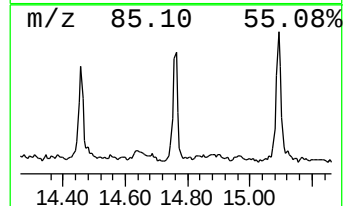
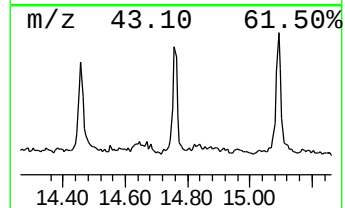
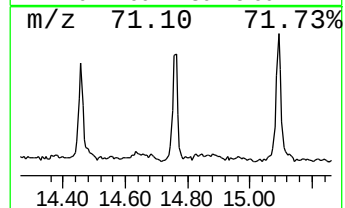
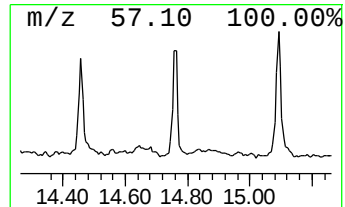
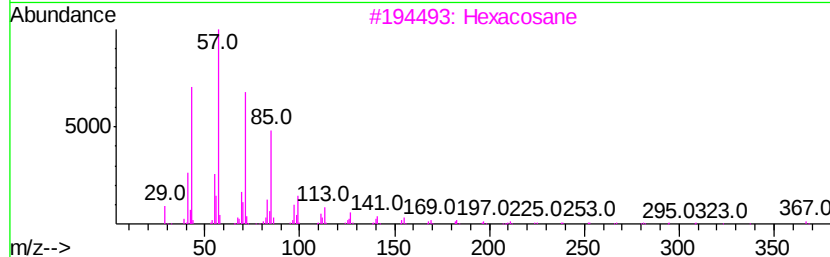
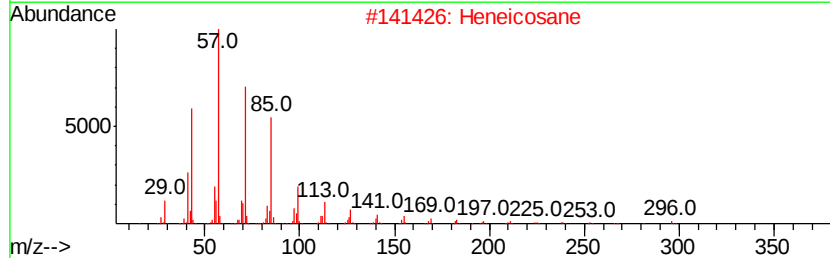
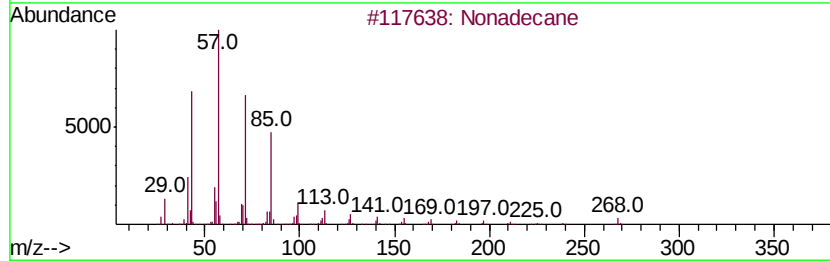
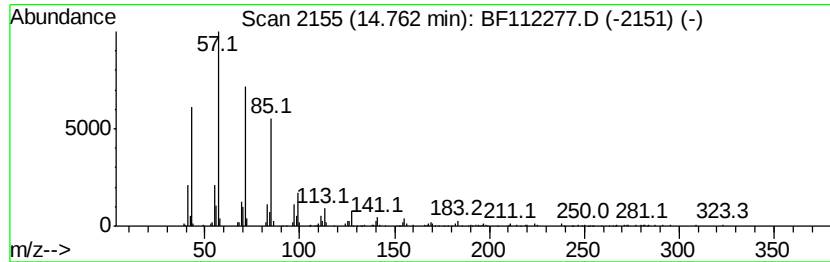
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	3.00 ng	267870	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	95
2		Heneicosane	296	C21H44	000629-94-7	90
3		Hexacosane	366	C26H54	000630-01-3	90
4		2-methyloctacosane	408	C29H60	1000376-72-8	90
5		Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
 Data File : BF112277.D
 Acq On : 28 Jan 2019 16:25
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 Sample : K1261-03
 Misc :
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Instrument :
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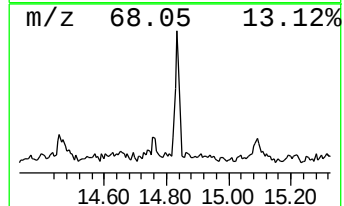
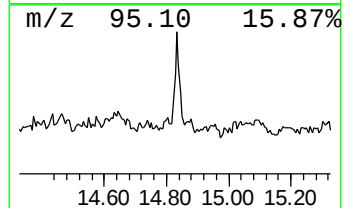
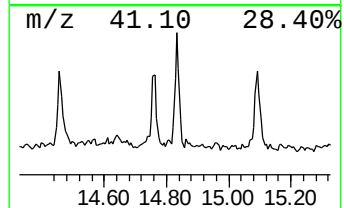
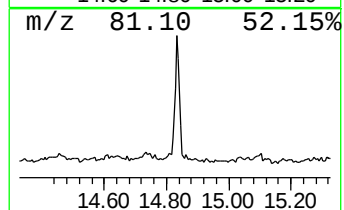
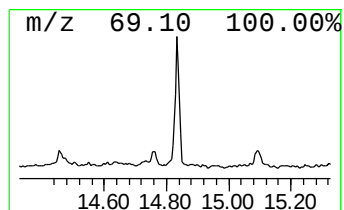
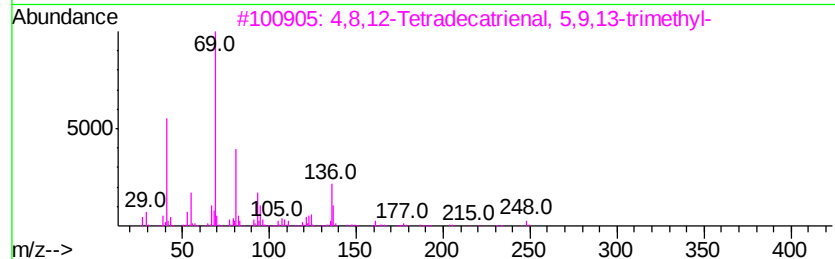
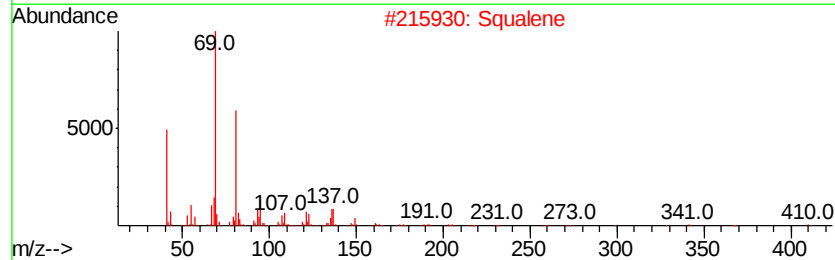
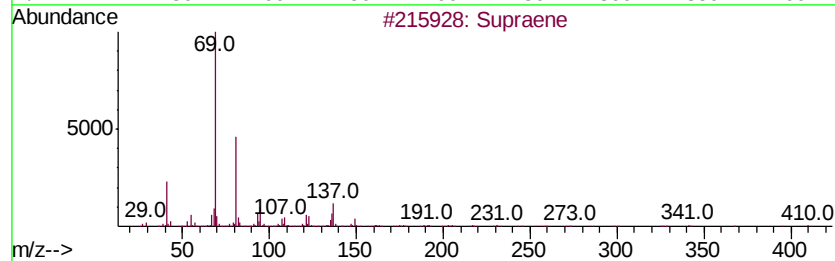
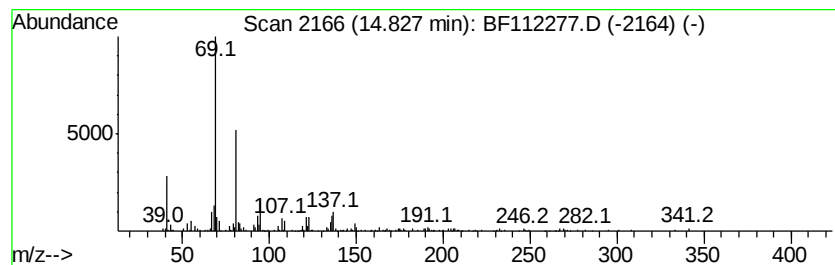
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.27 ng	291690	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	86
4		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
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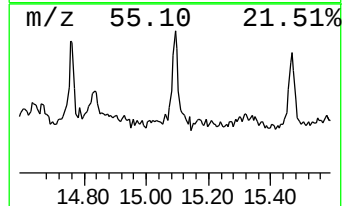
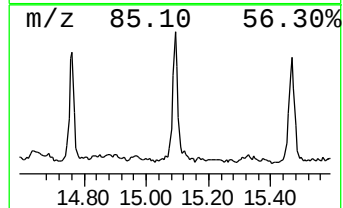
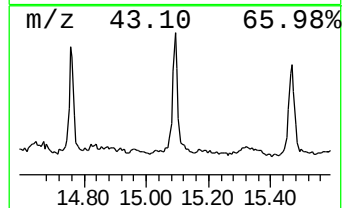
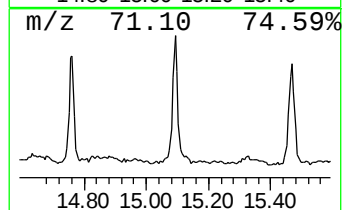
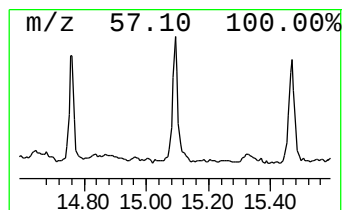
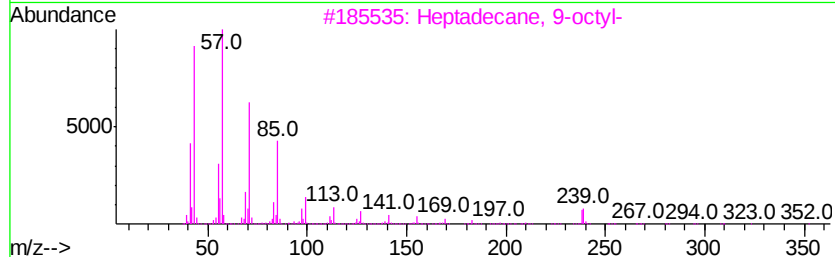
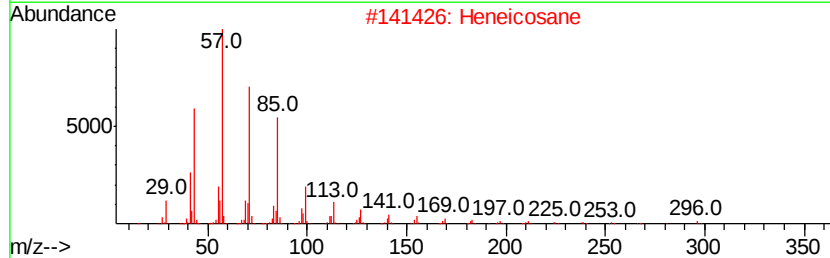
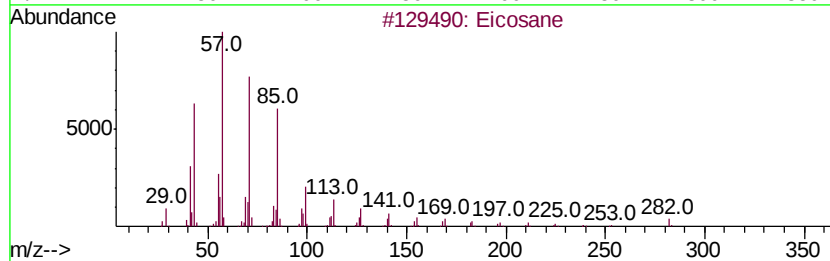
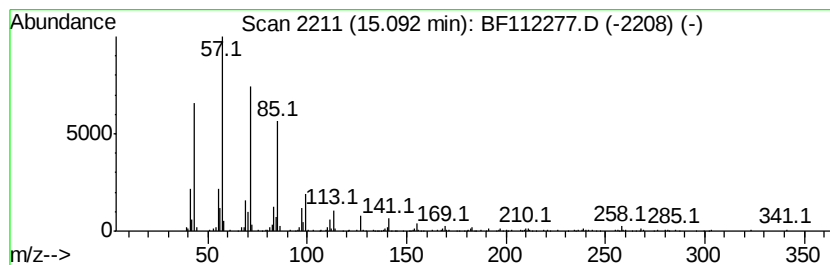
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	4.79 ng	427711	Perylene-d12	15.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	93
2	Heneicosane	296 C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
4	Docosane, 11-butyl-	366 C26H54	013475-76-8	91
5	Pentacosane	352 C25H52	000629-99-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
Data File : BF112277.D
Acq On : 28 Jan 2019 16:25
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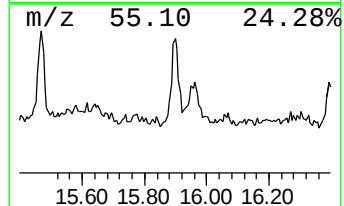
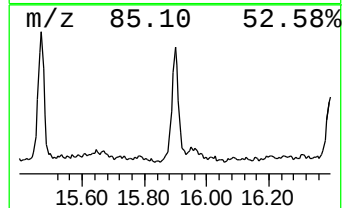
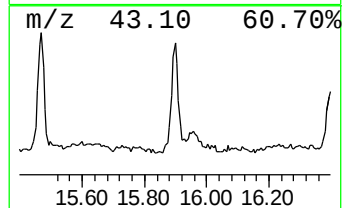
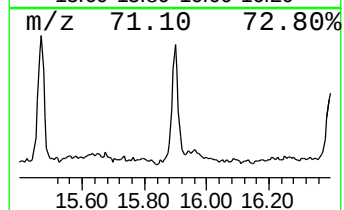
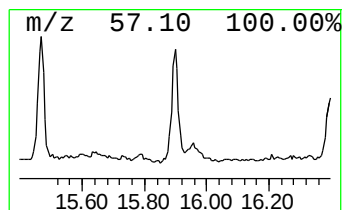
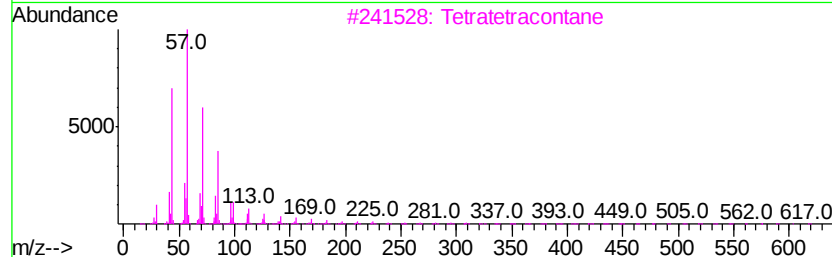
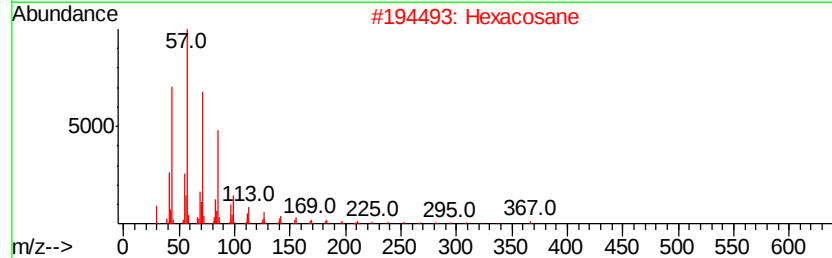
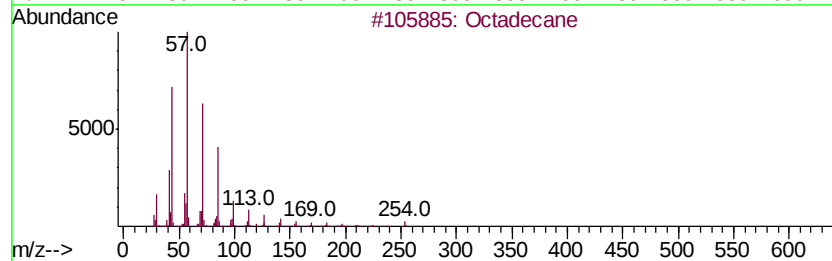
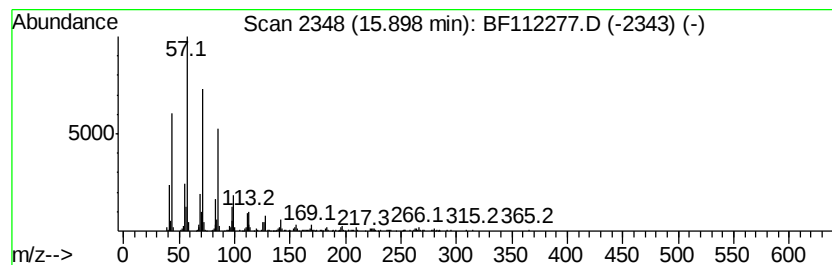
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.90	4.47 ng	399344	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	96
2	Hexacosane		366	C26H54	000630-01-3	91
3	Tetratetracontane		619	C44H90	007098-22-8	91
4	2-methyloctacosane		408	C29H60	1000376-72-8	91
5	Tetracosane		338	C24H50	000646-31-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012819\
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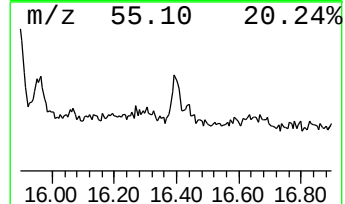
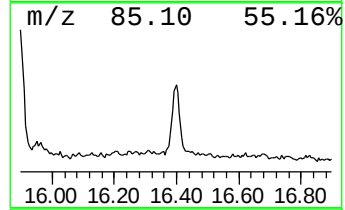
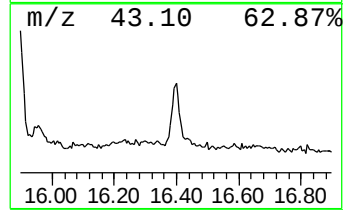
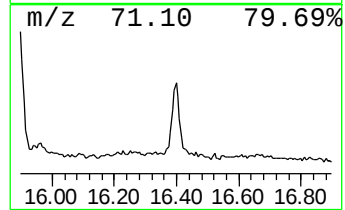
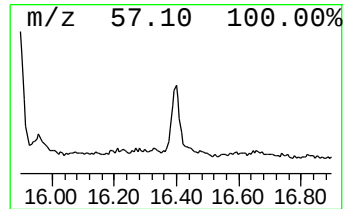
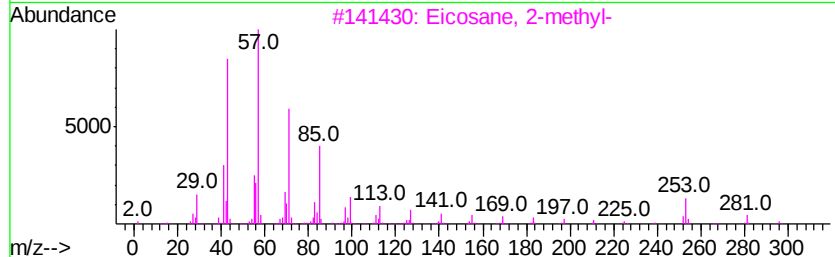
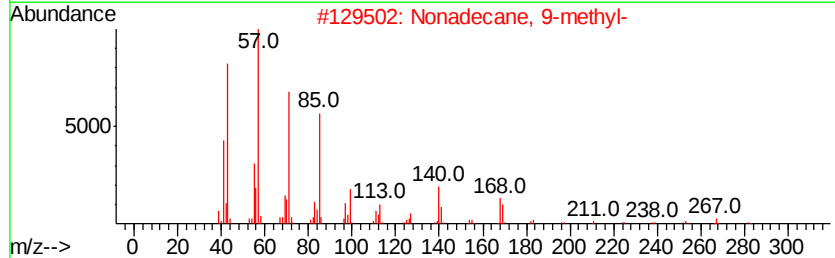
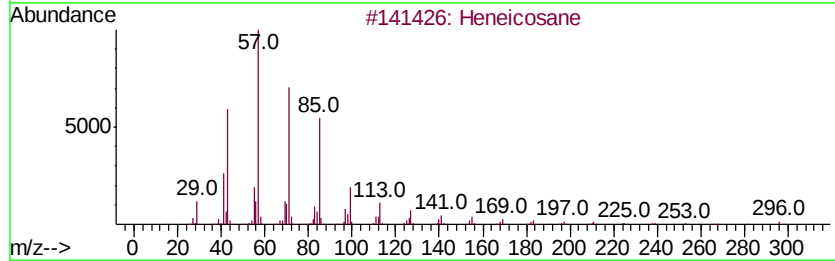
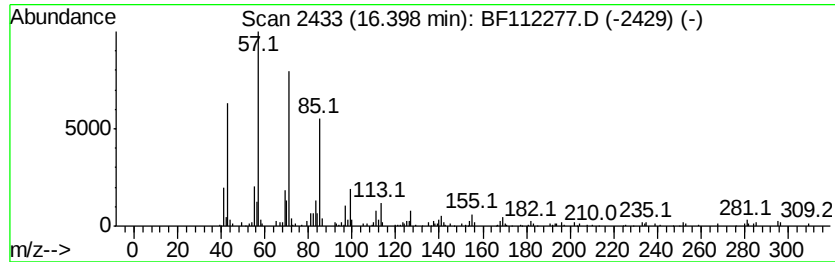
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.09 ng	186531	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	96
2		Nonadecane, 9-methyl-	282	C20H42	013287-24-6	95
3		Eicosane, 2-methyl-	296	C21H44	001560-84-5	94
4		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
5		Nonadecane	268	C19H40	000629-92-5	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012819\
Data File : BF112277.D
Acq On : 28 Jan 2019 16:25
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Sample : K1261-03
Misc :
ALS Vial : 16 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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2-Pentanone, 4-hy...	5.08	4.8	ng	319047	1	6.84	1320520	20.0
unknown6.62	6.62	95.2	ng	6282630	1	6.84	1320520	20.0
n-Hexadecanoic acid	11.89	5.1	ng	575899	4	11.36	2247890	20.0
5-Eicosene, (E)-	13.83	9.8	ng	1035140	5	14.00	2121790	20.0
Tetracosane	14.46	3.2	ng	339734	5	14.00	2121790	20.0
Nonadecane	14.76	3.0	ng	267870	6	15.47	1785520	20.0
Supraene	14.83	3.3	ng	291690	6	15.47	1785520	20.0
Eicosane	15.09	4.8	ng	427711	6	15.47	1785520	20.0
Octadecane	15.90	4.5	ng	399344	6	15.47	1785520	20.0
Heneicosane	16.40	2.1	ng	186531	6	15.47	1785520	20.0