

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021919\
 Data File : BF112628.D
 Acq On : 19 Feb 2019 18:37
 Operator : JU/SJ
 Sample : K1515-14
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TS-14

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	5.045	499	503	517	rBV	62506	100576	3.68%	0.434%
2	5.457	569	573	597	rBV	2039391	2166727	79.26%	9.344%
3	6.475	742	746	763	rBV	2148365	2308603	84.45%	9.956%
4	6.598	763	767	780	rVB	2740253	2463437	90.12%	10.623%
5	6.822	801	805	814	rBV	508922	459527	16.81%	1.982%
6	6.975	827	831	849	rBV	1966726	1851691	67.74%	7.985%
7	7.386	897	901	925	rBV	1423988	1461863	53.48%	6.304%
8	8.104	1019	1023	1039	rBV	566066	586348	21.45%	2.529%
9	9.174	1201	1205	1216	rBV	2985983	2724309	99.66%	11.748%
10	9.574	1269	1273	1287	rVB	98276	99184	3.63%	0.428%
11	9.857	1317	1321	1333	rVB2	718705	687727	25.16%	2.966%
12	10.651	1452	1456	1482	rBV	1789380	1951356	71.38%	8.415%
13	11.351	1571	1575	1588	rBV	664547	722134	26.42%	3.114%
14	11.863	1659	1662	1678	rBV2	213845	268221	9.81%	1.157%
15	12.574	1777	1783	1793	rBV	17511	31403	1.15%	0.135%
16	12.651	1793	1796	1804	rBV5	32086	49389	1.81%	0.213%
17	12.927	1838	1843	1846	rBV	3060120	2733633	100.00%	11.789%
18	13.139	1875	1879	1885	rBV3	20492	30250	1.11%	0.130%
19	13.809	1989	1993	2005	rBV	291834	442962	16.20%	1.910%
20	13.992	2020	2024	2032	rBV	635512	626870	22.93%	2.703%
21	14.127	2043	2047	2050	rBV	36670	37096	1.36%	0.160%
22	14.433	2095	2099	2101	rBV	61214	67544	2.47%	0.291%
23	14.457	2101	2103	2112	rVB4	28462	44990	1.65%	0.194%
24	14.733	2145	2150	2153	rVB	64984	73622	2.69%	0.317%
25	14.804	2158	2162	2166	rVV	126988	118678	4.34%	0.512%
26	15.062	2201	2206	2209	rBV2	88644	103048	3.77%	0.444%
27	15.433	2265	2269	2271	rBV	54416	66434	2.43%	0.286%
28	15.468	2271	2275	2285	rVB	397126	539272	19.73%	2.326%
29	15.856	2336	2341	2346	rBV2	57270	84936	3.11%	0.366%
30	15.933	2348	2354	2362	rBV10	32861	92281	3.38%	0.398%
31	16.345	2420	2424	2428	rBV3	27922	49268	1.80%	0.212%
32	16.386	2428	2431	2440	rVB	30046	55395	2.03%	0.239%
33	16.927	2516	2523	2528	rBV7	17668	37803	1.38%	0.163%
34	17.192	2564	2568	2576	rVB9	22668	52249	1.91%	0.225%

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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-BF012519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

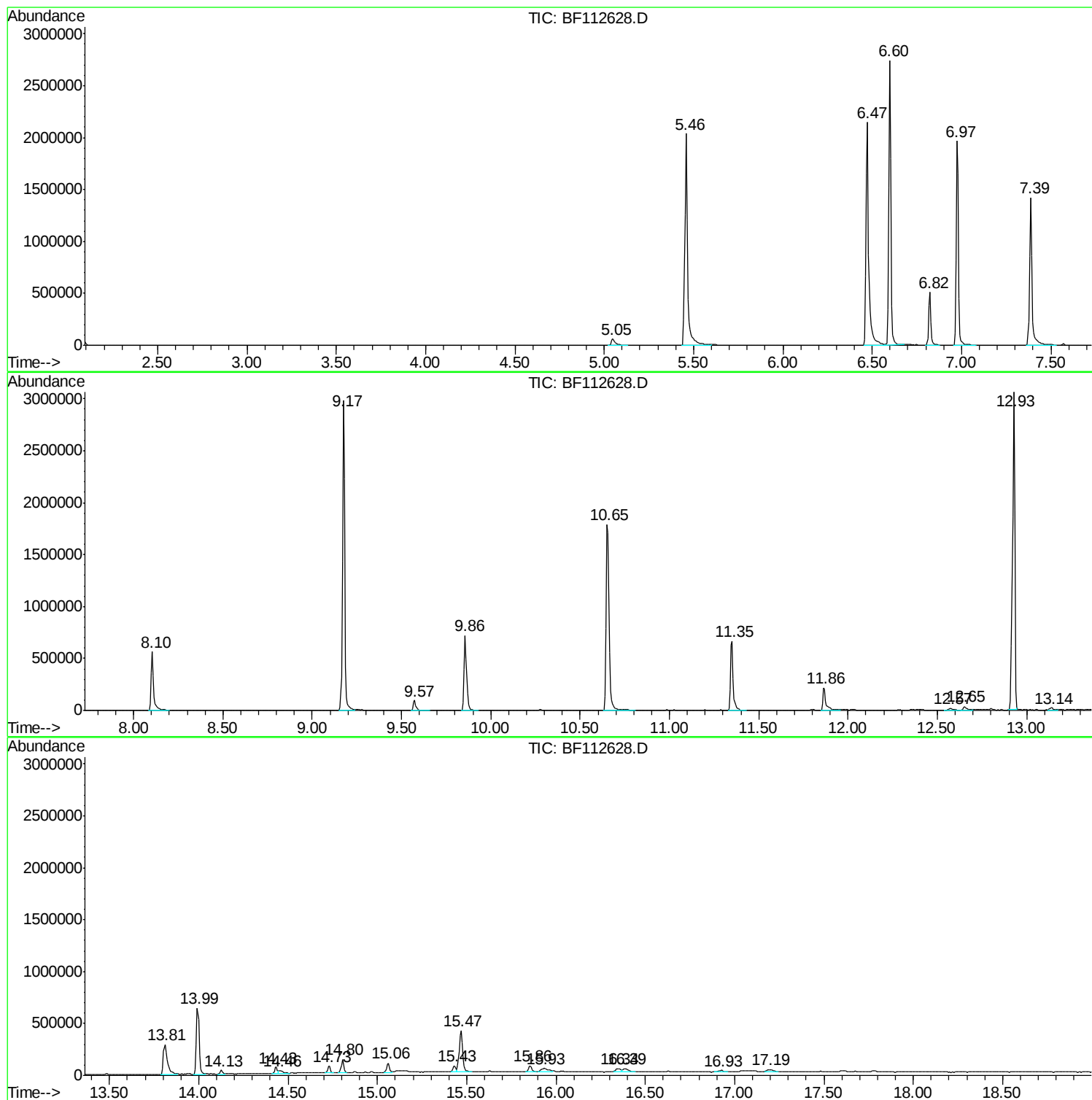
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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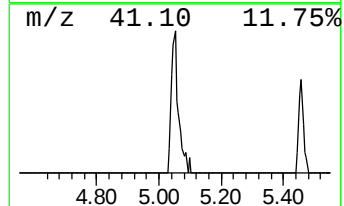
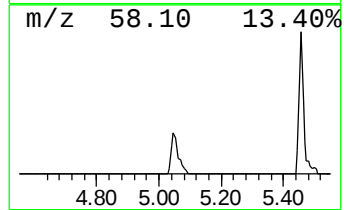
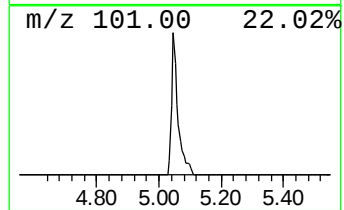
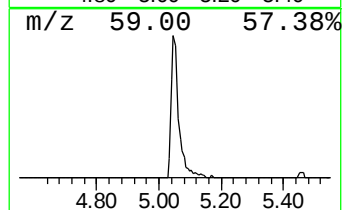
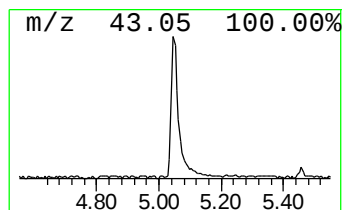
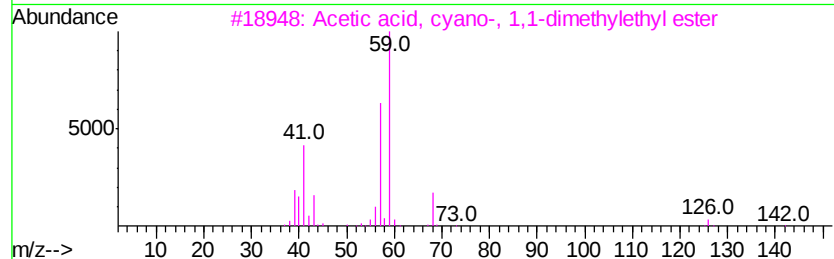
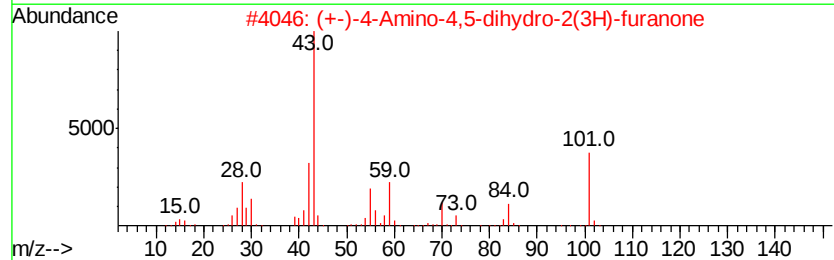
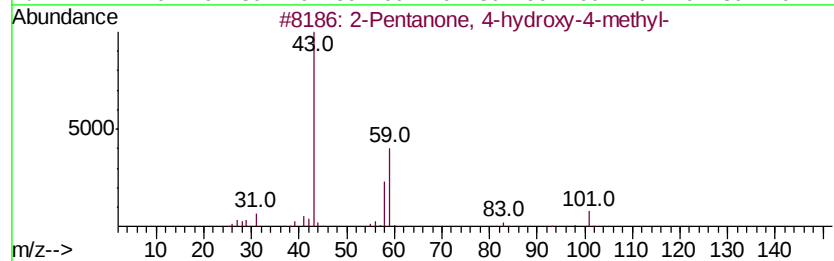
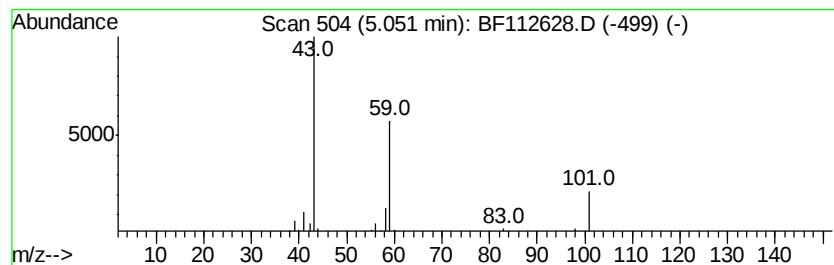
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	4.38 ng	100576	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	72
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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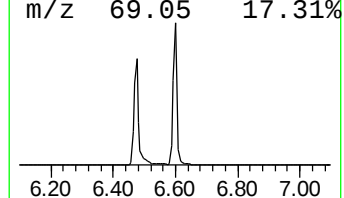
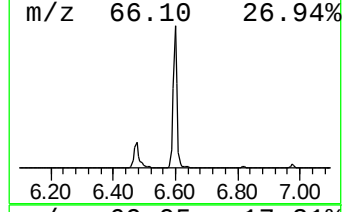
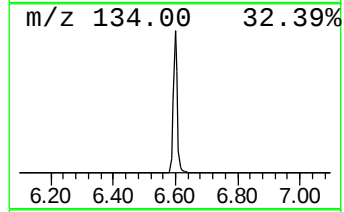
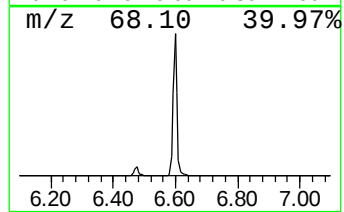
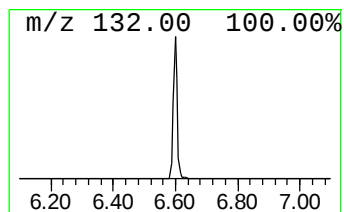
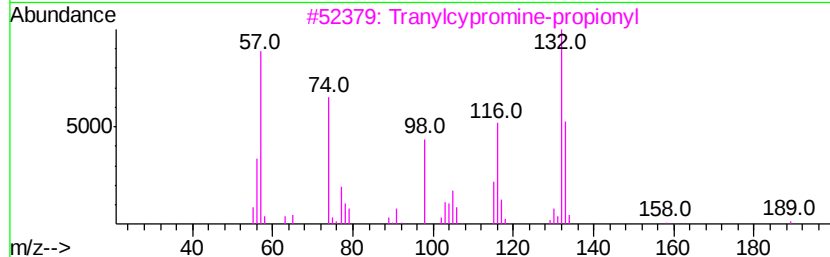
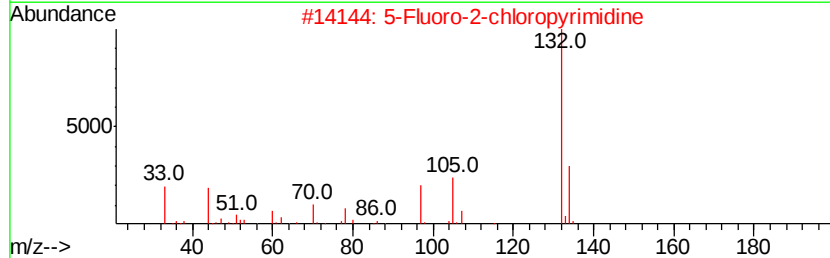
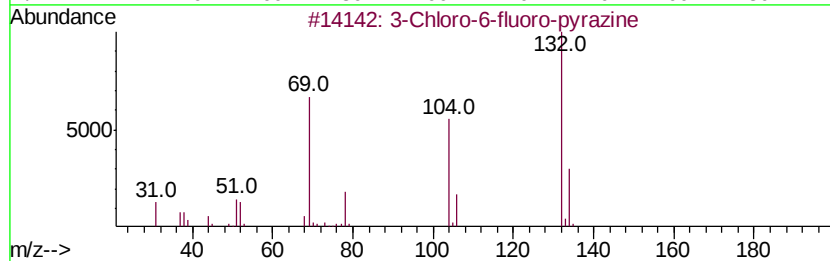
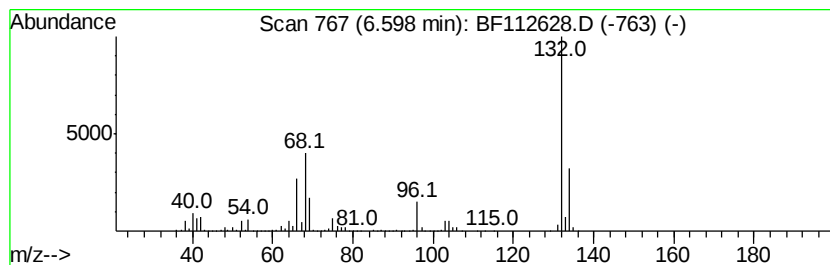
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	107.22 ng	2463440	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Xenon	132	Xe	007440-63-3	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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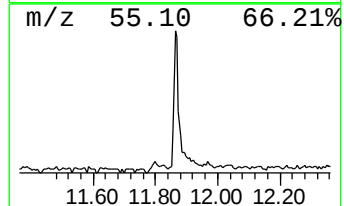
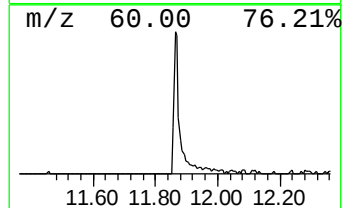
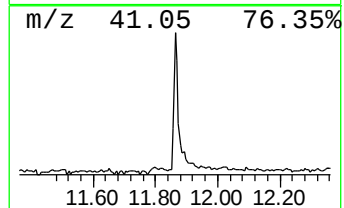
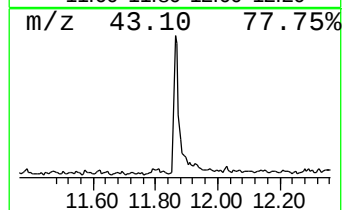
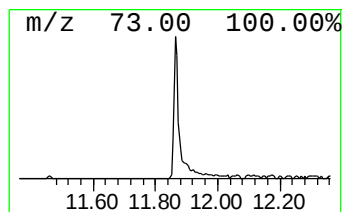
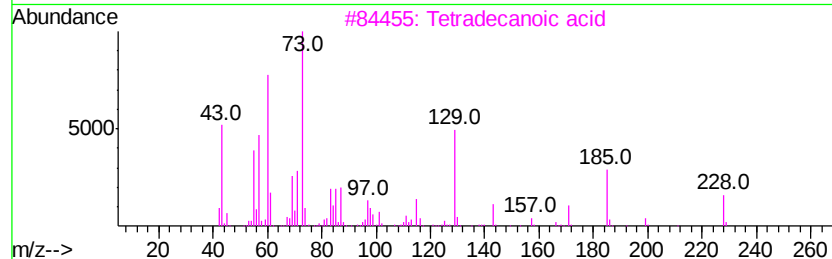
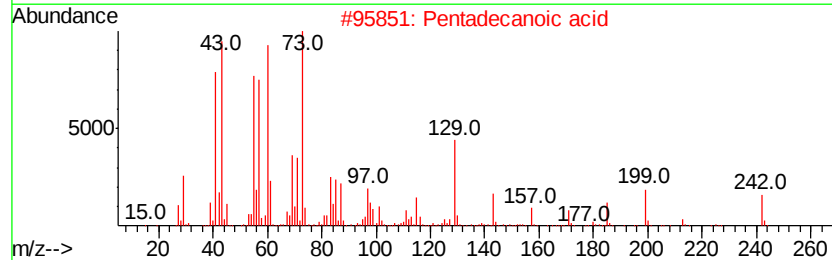
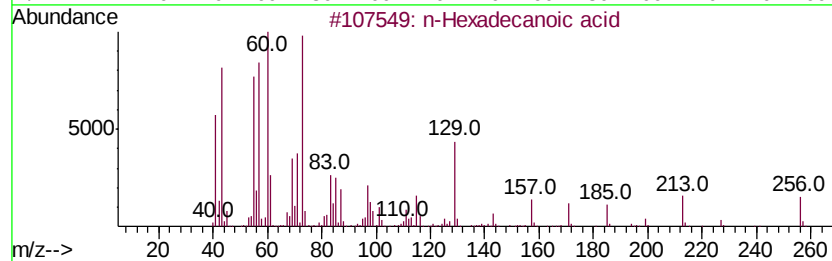
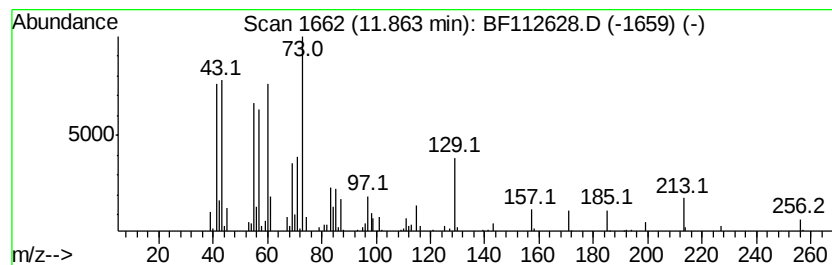
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	7.43 ng	268221	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



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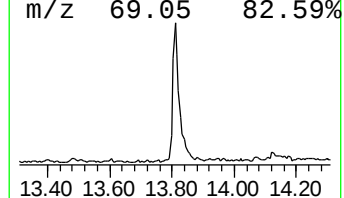
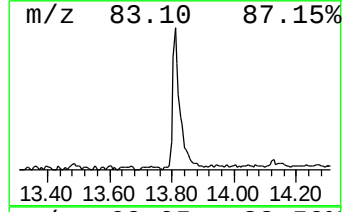
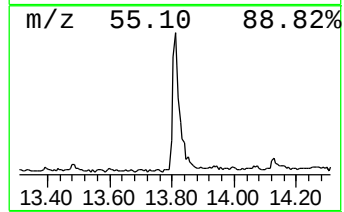
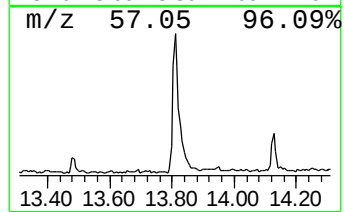
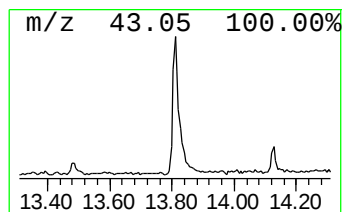
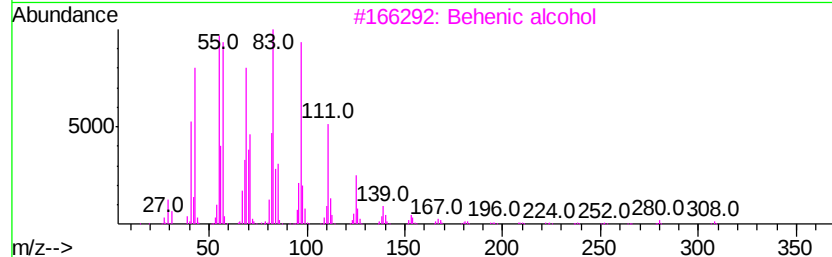
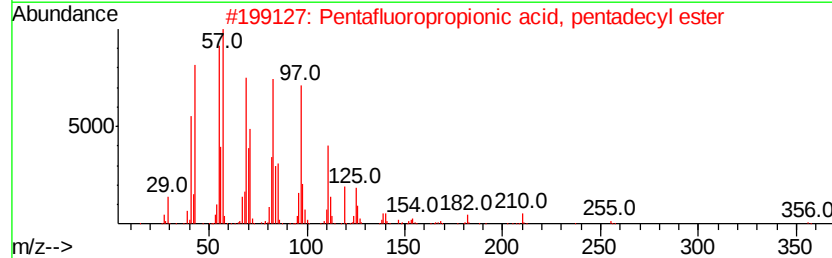
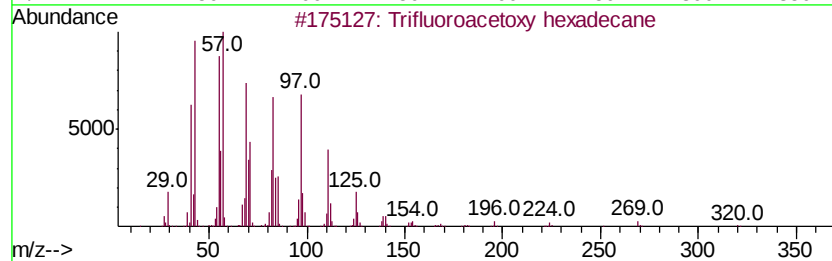
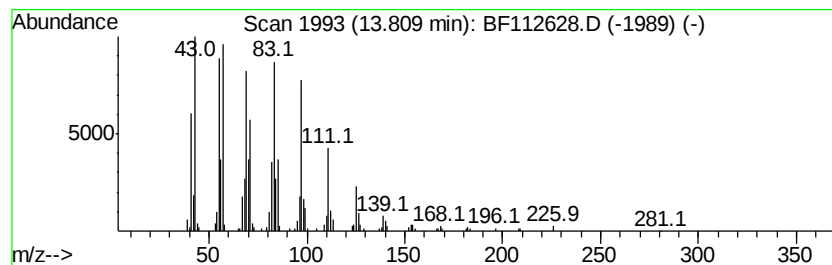
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	14.13 ng	442962	Chrysene-d12	13.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



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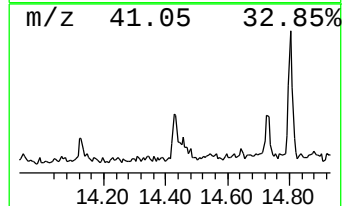
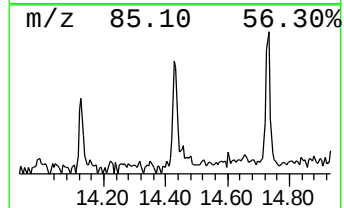
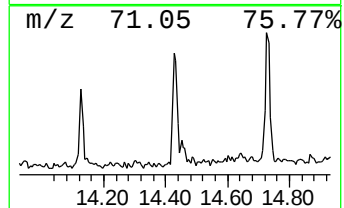
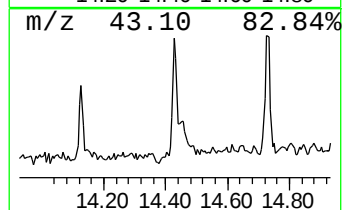
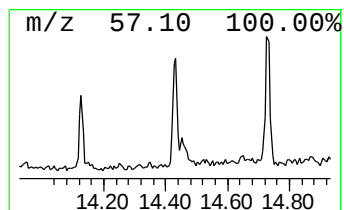
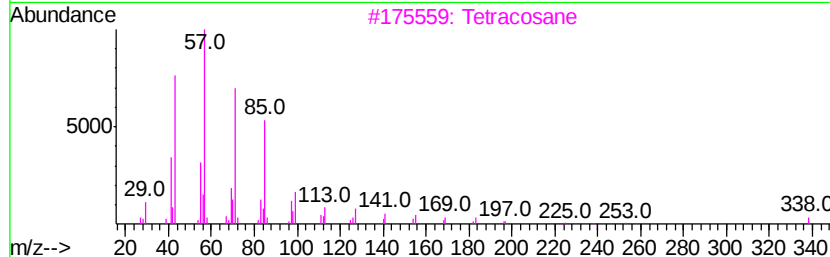
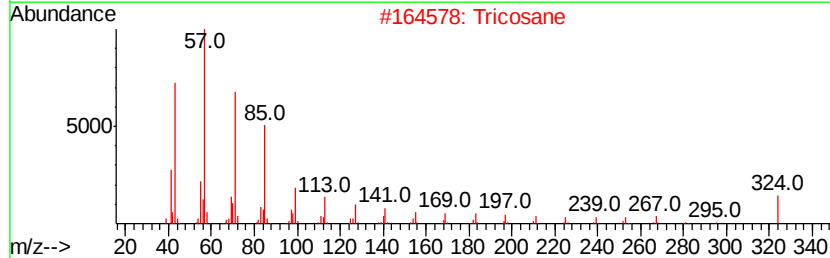
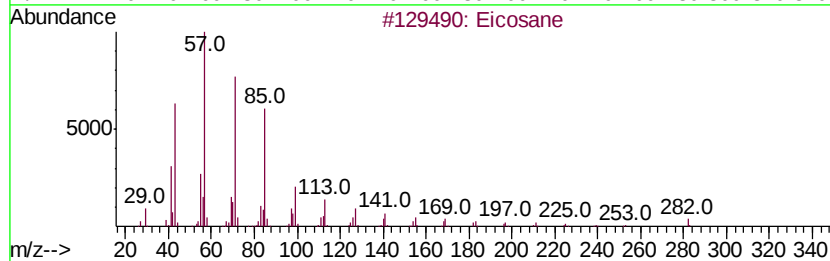
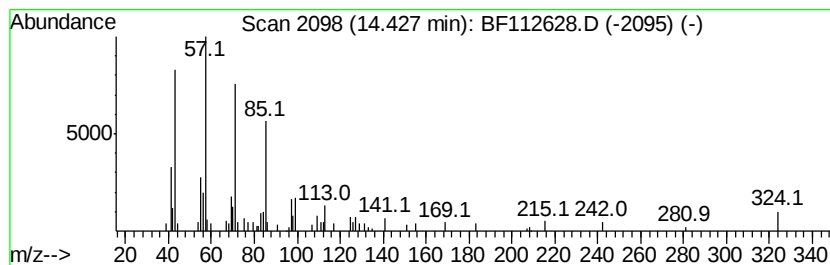
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Peak Number 6 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.43	2.15 ng	67544	Chrysene-d12		13.99
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Tricosane	324	C23H48	000638-67-5	95
3	Tetracosane	338	C24H50	000646-31-1	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	87



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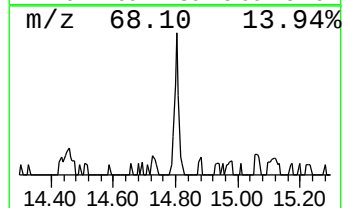
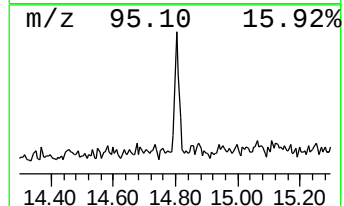
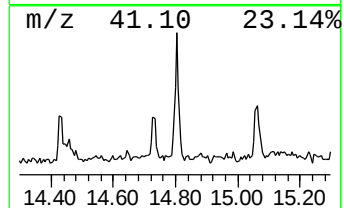
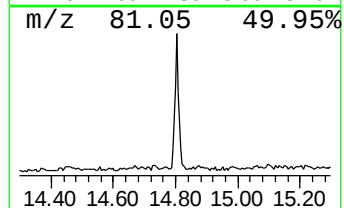
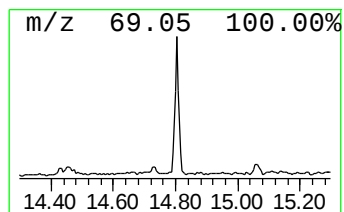
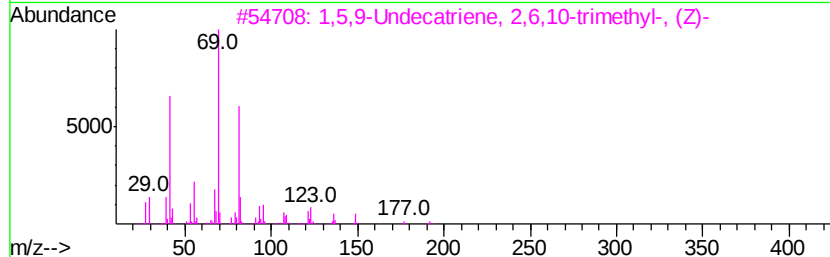
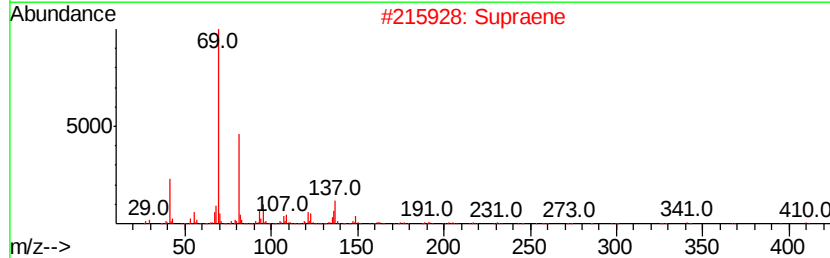
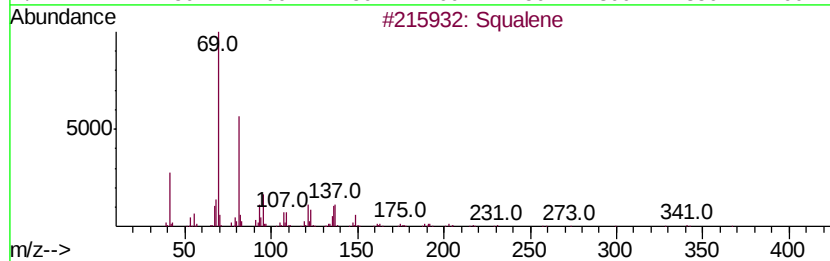
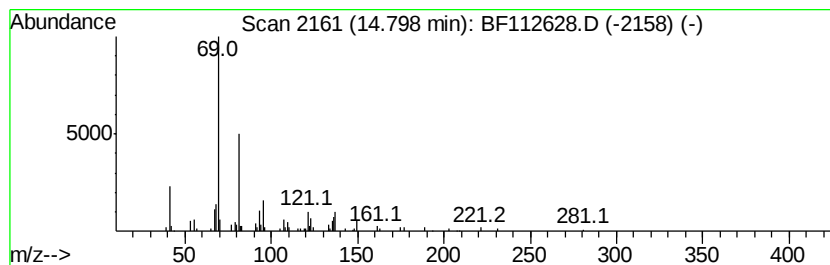
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.40 ng	118678	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		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	87
4		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
5		trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
Data File : BF112628.D
Acq On : 19 Feb 2019 18:37
Operator : JU/SJ
Sample : K1515-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-14

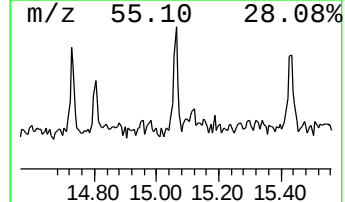
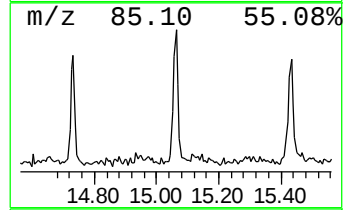
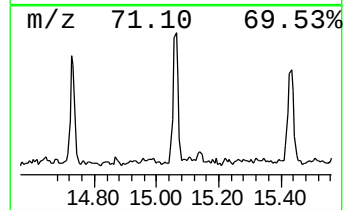
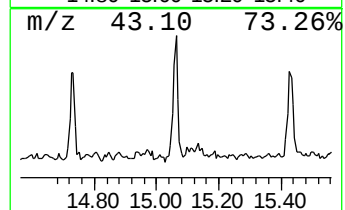
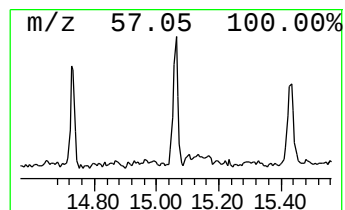
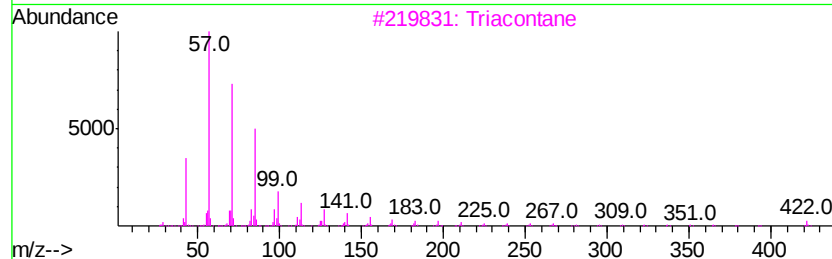
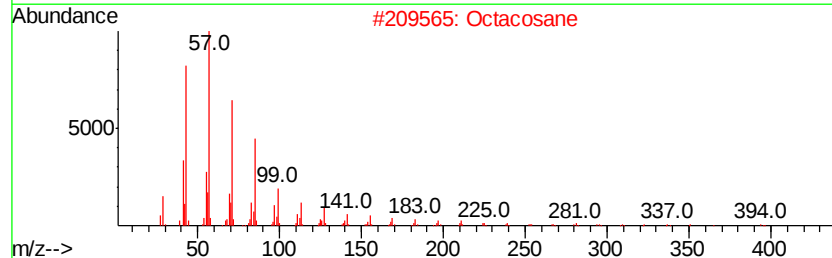
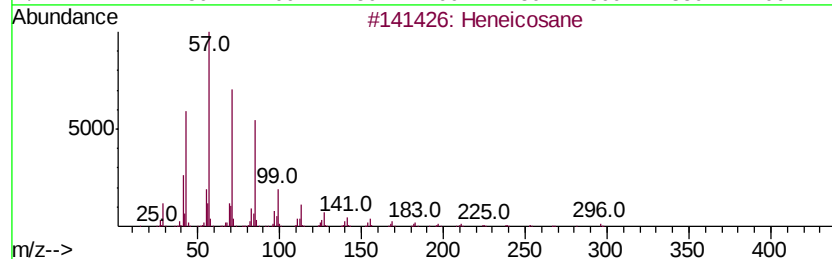
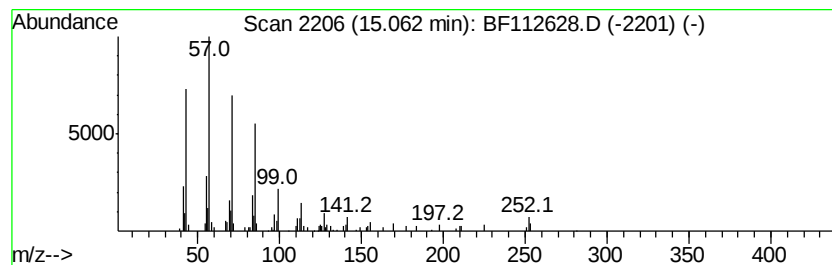
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	3.82 ng	103048	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Octacosane		394	C28H58	000630-02-4	90
3	Triacontane		422	C30H62	000638-68-6	90
4	2-methyloctacosane		408	C29H60	1000376-72-8	87
5	Tridecane, 3-methyl-		198	C14H30	006418-41-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
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Operator : JU/SJ
Sample : K1515-14
Misc :
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Instrument :
BNA_F
ClientSampleId :
TS-14

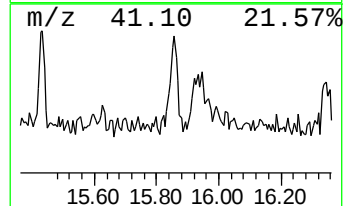
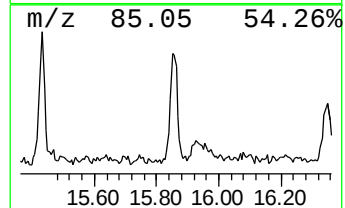
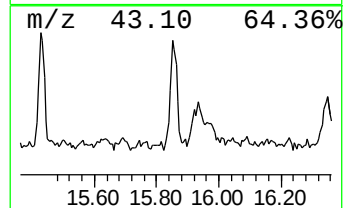
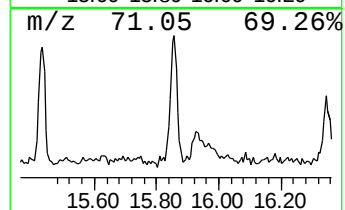
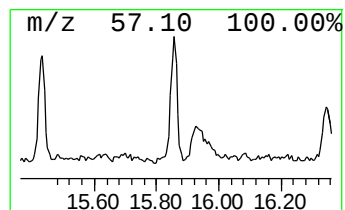
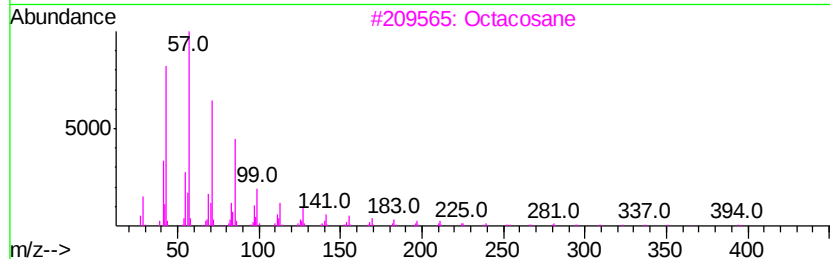
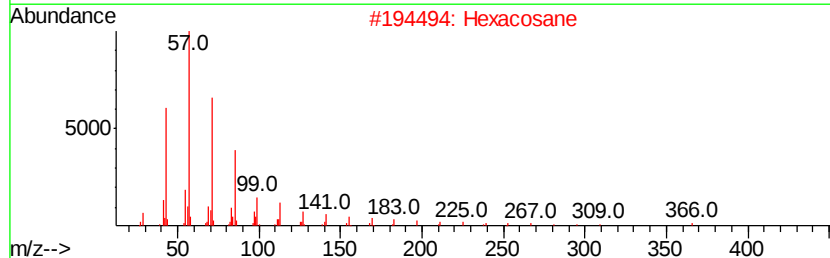
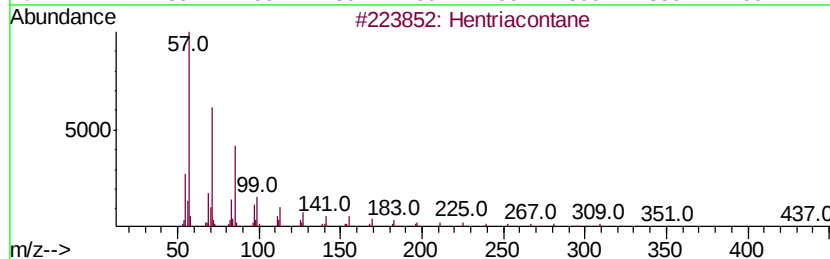
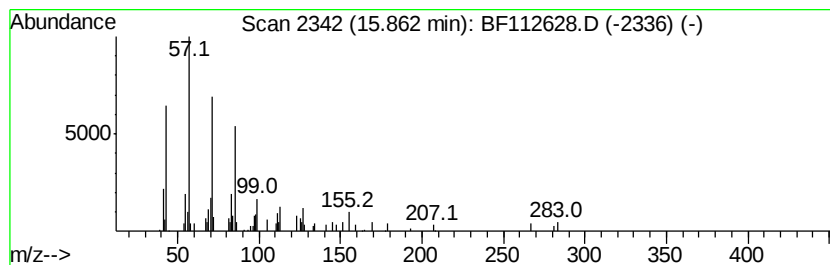
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.15 ng	84936	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Hexacosane		366	C26H54	000630-01-3	91
3	Octacosane		394	C28H58	000630-02-4	90
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	90
5	Tetratetracontane		619	C44H90	007098-22-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
Data File : BF112628.D
Acq On : 19 Feb 2019 18:37
Operator : JU/SJ
Sample : K1515-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TS-14

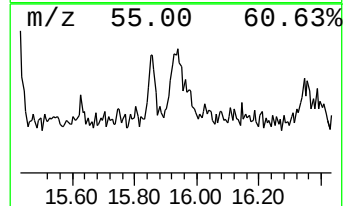
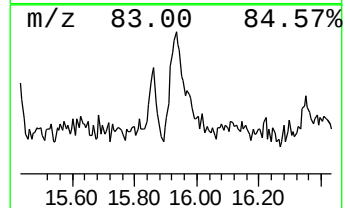
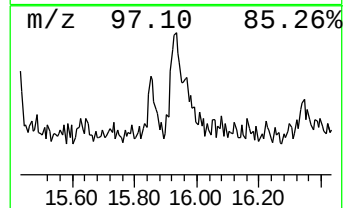
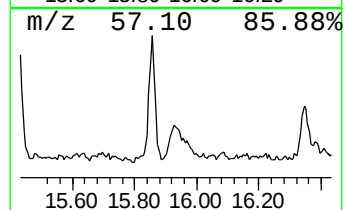
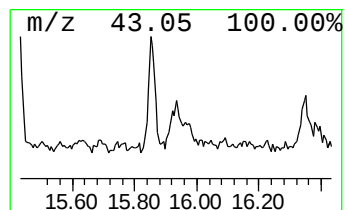
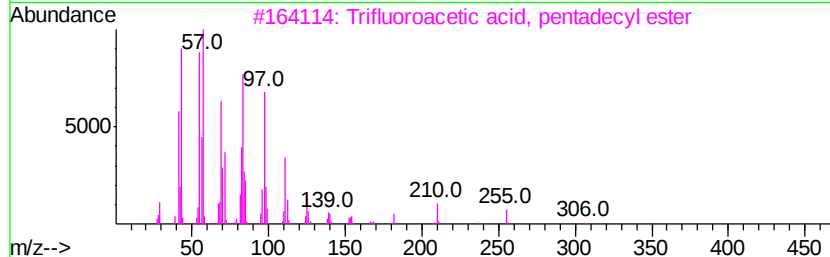
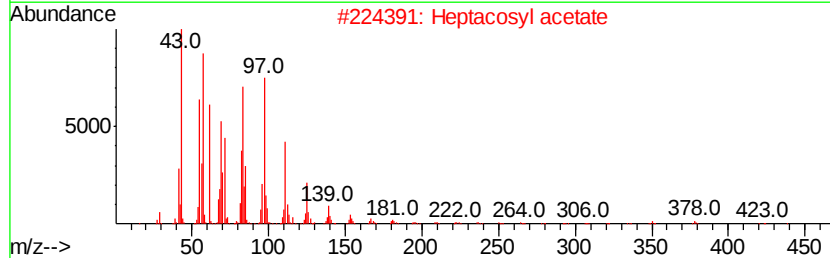
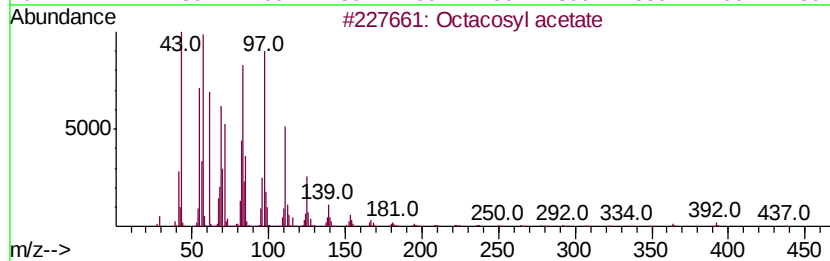
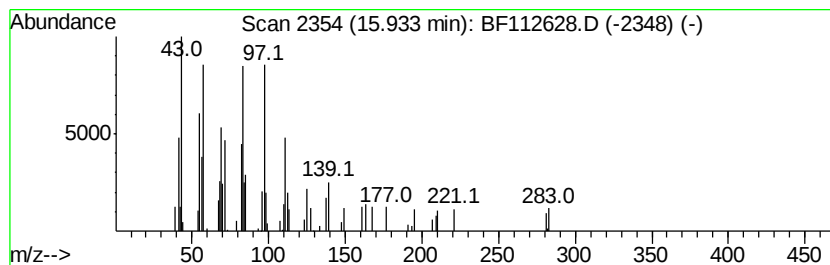
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	3.42 ng	92281	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosyl acetate	452	C30H60O2	018206-97-8	87
2		Heptacosyl acetate	438	C29H58O2	1000351-78-2	87
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
4		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	86
5		1-Heneicosanol	312	C21H44O	015594-90-8	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF021919\
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Acq On : 19 Feb 2019 18:37
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Sample : K1515-14
Misc :
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ClientSampleId :
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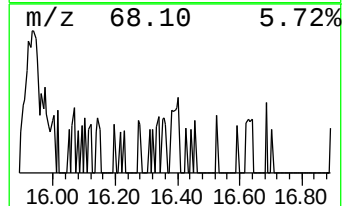
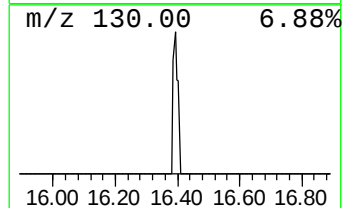
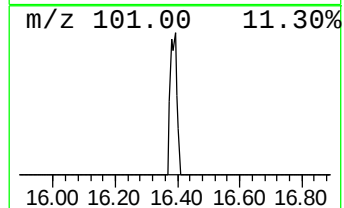
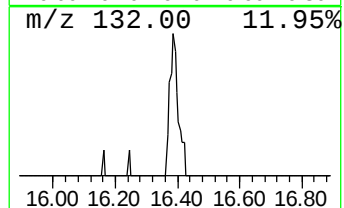
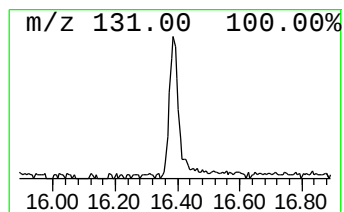
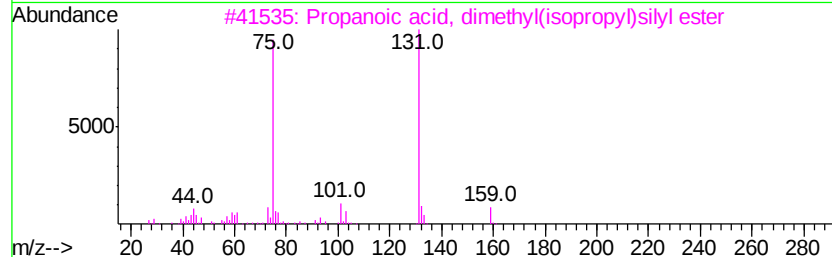
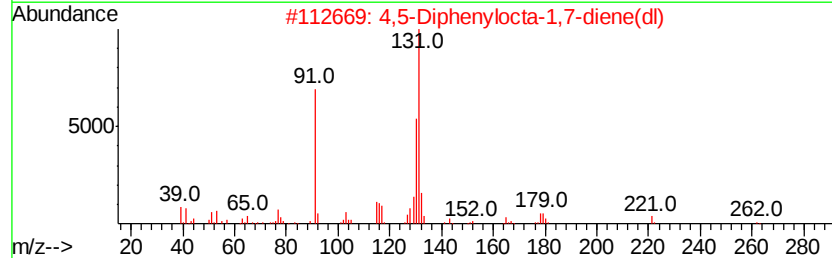
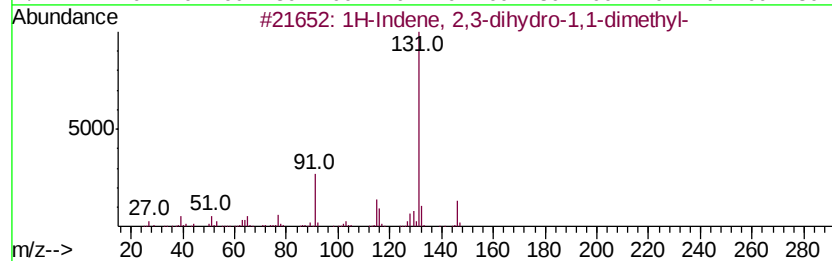
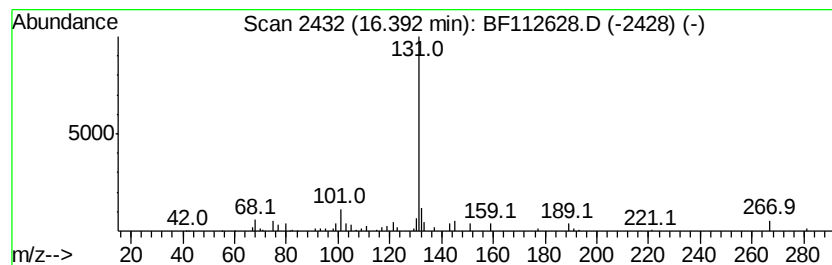
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.39 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.39	2.05 ng	55395	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-1,1-dimet...	146	C11H14	004912-92-9	38
2		4,5-Diphenylocta-1,7-diene(dl)	262	C20H22	1000215-92-8	38
3		Propanoic acid, dimethyl(isoprop...	174	C8H18O2Si	1000279-45-8	36
4		Pyrido[2,3-b]pyrazine	131	C7H5N3	000322-46-3	9
5		Pyrido[2,3-d]pyrimidine	131	C7H5N3	000254-61-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF021919\
Data File : BF112628.D
Acq On : 19 Feb 2019 18:37
Operator : JU/SJ
Sample : K1515-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
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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unknown6.60	6.60	107.2	ng	2463440	1	6.82	459527	20.0
n-Hexadecanoic acid	11.86	7.4	ng	268221	4	11.35	722134	20.0
Trifluoroacetoxy ...	13.81	14.1	ng	442962	5	13.99	626870	20.0
Eicosane	14.43	2.1	ng	67544	5	13.99	626870	20.0
Squalene	14.80	4.4	ng	118678	6	15.47	539272	20.0
Heneicosane	15.06	3.8	ng	103048	6	15.47	539272	20.0
Hentriacontane	15.86	3.1	ng	84936	6	15.47	539272	20.0
Octacosyl acetate	15.93	3.4	ng	92281	6	15.47	539272	20.0
unknown16.39	16.39	2.0	ng	55395	6	15.47	539272	20.0