

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072919\
 Data File : BF115836.D
 Acq On : 29 Jul 2019 17:07
 Operator : HP/JU
 Sample : K4036-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WS-04

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-BF071219.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	2.140	3	9	41	rVB	2749303	3980619	89.74%	10.776%
2	5.075	503	508	524	rVB	636573	750113	16.91%	2.031%
3	5.481	573	577	599	rBV	2328666	2335471	52.65%	6.322%
4	6.487	744	748	768	rBV	1941528	1915620	43.19%	5.186%
5	6.634	768	773	776	rBV	3417941	3216994	72.53%	8.708%
6	6.857	808	811	815	rBV	950497	844620	19.04%	2.286%
7	7.016	834	838	842	rBV	3046015	2847420	64.20%	7.708%
8	7.422	902	907	910	rBV	2418974	2285890	51.54%	6.188%
9	8.139	1025	1029	1042	rBV	1186800	1067234	24.06%	2.889%
10	9.216	1207	1212	1215	rBV	4498681	4185855	94.37%	11.331%
11	9.604	1275	1278	1283	rBV	151407	137258	3.09%	0.372%
12	9.892	1323	1327	1336	rVB	1526332	1258539	28.37%	3.407%
13	10.680	1457	1461	1476	rBV	1671373	1548481	34.91%	4.192%
14	11.374	1576	1579	1588	rBV	1342808	1318451	29.72%	3.569%
15	11.539	1604	1607	1611	rVB2	73703	69977	1.58%	0.189%
16	11.933	1671	1674	1678	rVB	70770	62313	1.40%	0.169%
17	12.963	1844	1849	1852	rBV	4551774	4435507	100.00%	12.007%
18	13.857	1998	2001	2003	rBV	51835	48123	1.08%	0.130%
19	13.892	2003	2007	2021	rVV4	53702	175147	3.95%	0.474%
20	14.015	2024	2028	2034	rVB	1241918	1146414	25.85%	3.103%
21	14.174	2051	2055	2061	rBV	97629	85852	1.94%	0.232%
22	14.480	2102	2107	2112	rBV	180123	175664	3.96%	0.476%
23	14.786	2154	2159	2167	rBV	288835	316458	7.13%	0.857%
24	15.115	2211	2215	2224	rBV	372940	445196	10.04%	1.205%
25	15.480	2272	2277	2288	rBV2	748327	1427794	32.19%	3.865%
26	15.927	2347	2353	2367	rBV	289328	467559	10.54%	1.266%
27	16.433	2433	2439	2446	rBV	158298	285989	6.45%	0.774%
28	17.021	2533	2539	2547	rVB2	51543	106375	2.40%	0.288%

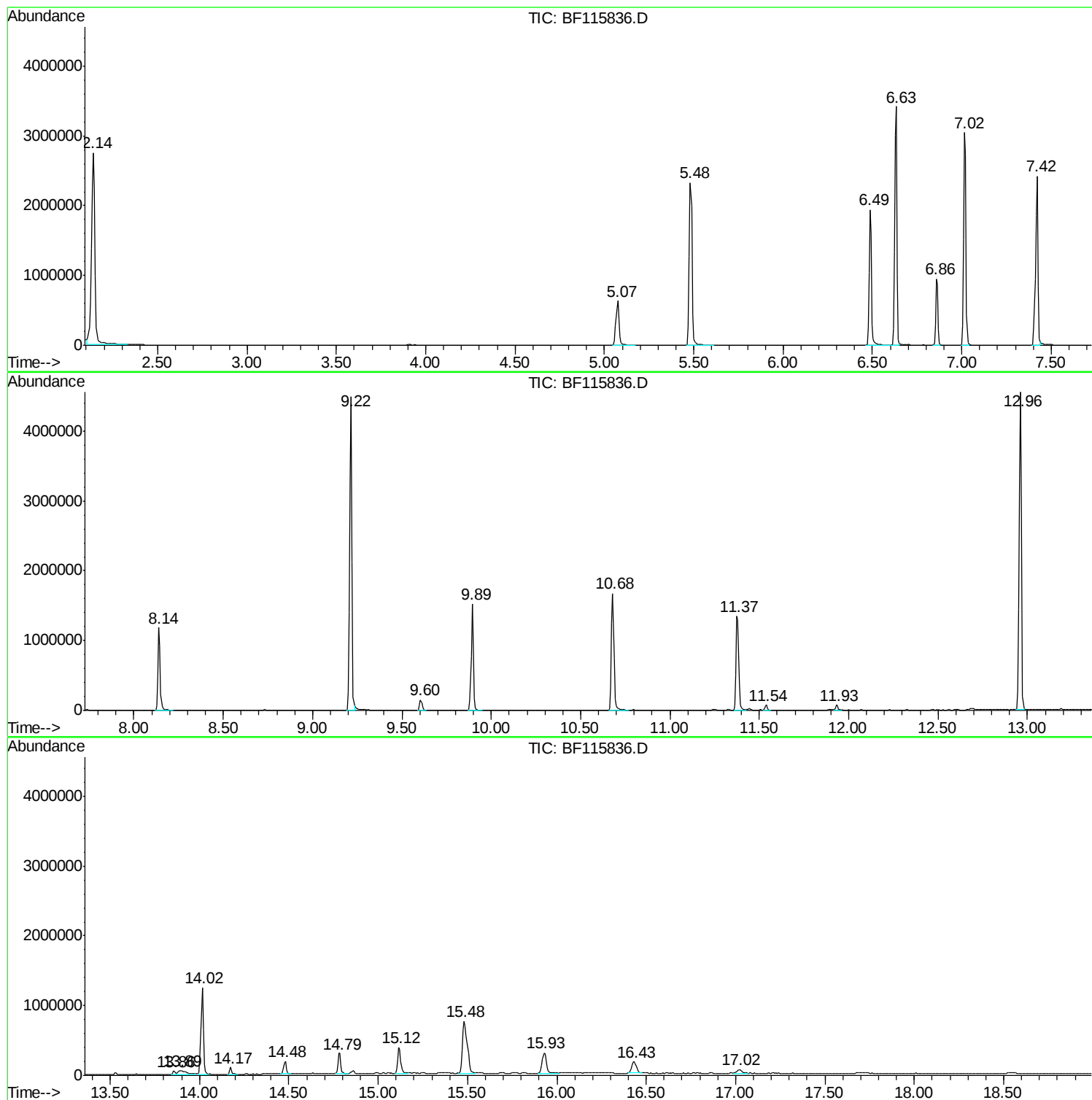
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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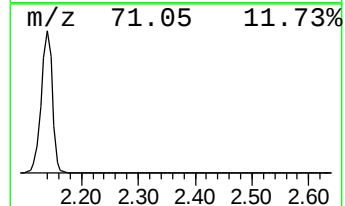
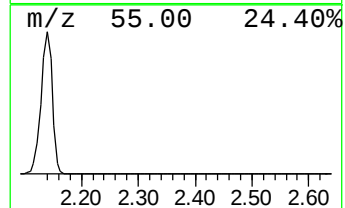
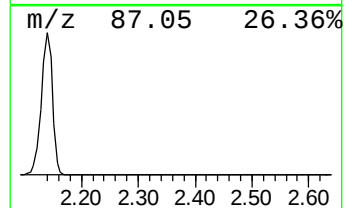
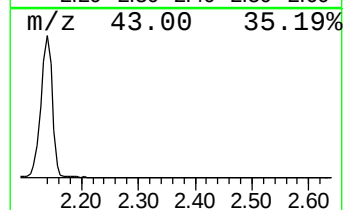
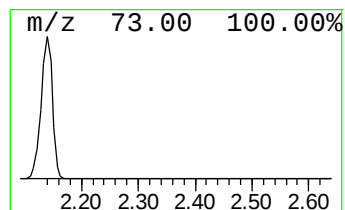
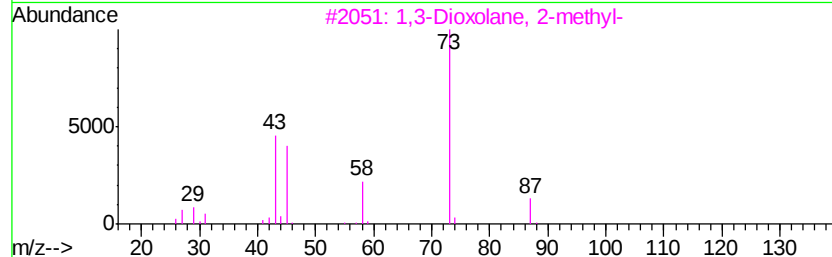
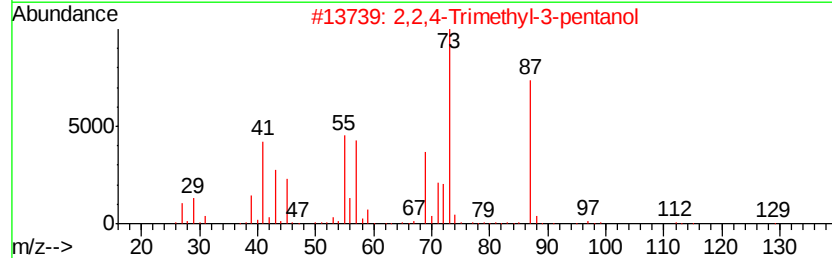
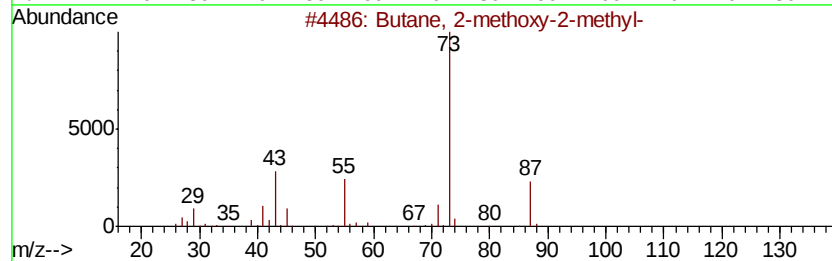
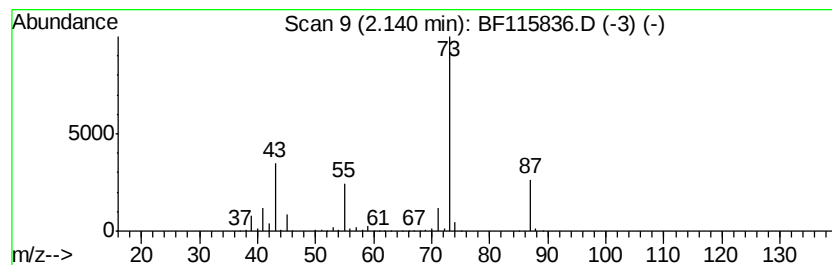
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	94.26 ng	3980620	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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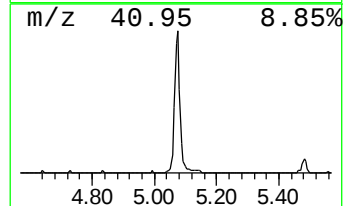
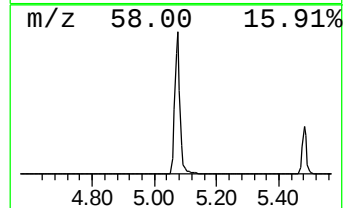
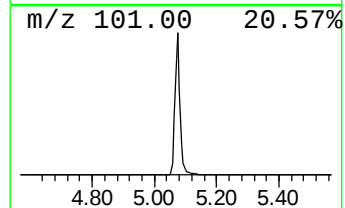
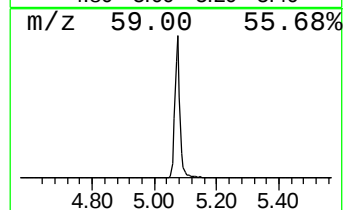
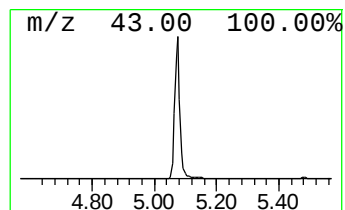
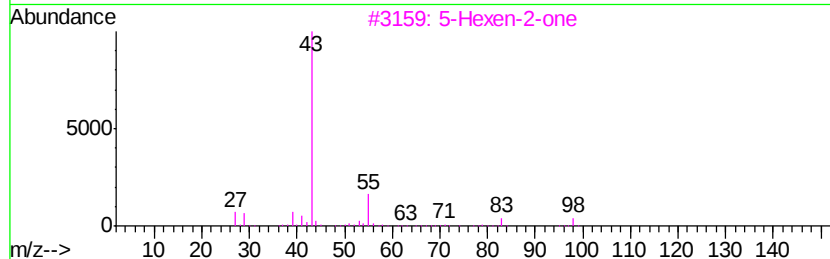
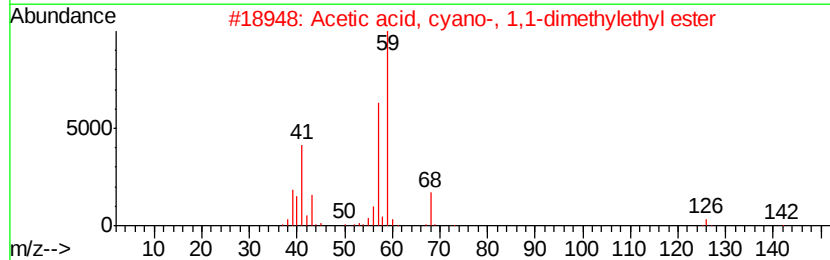
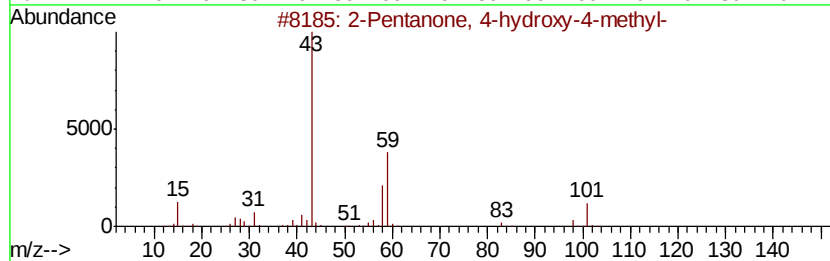
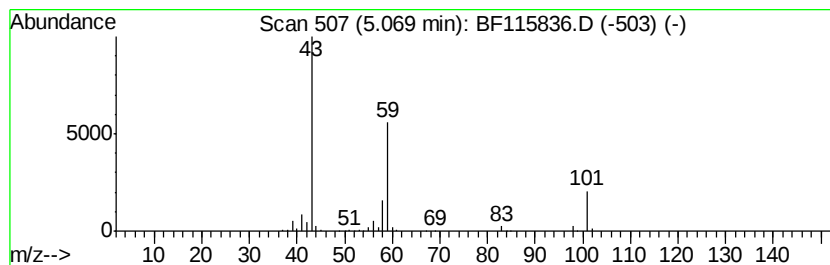
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	17.76 ng	750113	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



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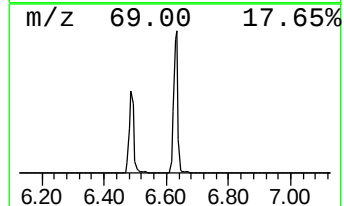
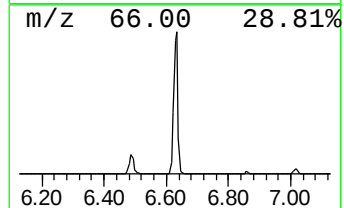
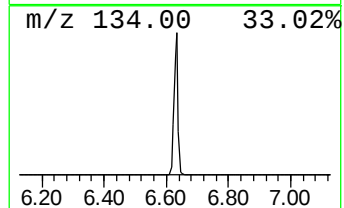
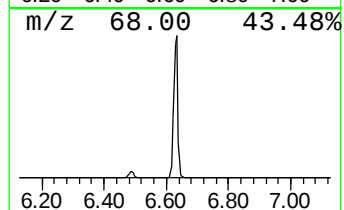
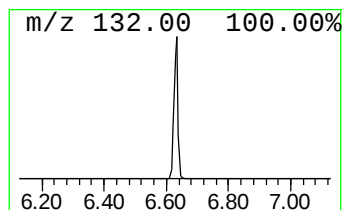
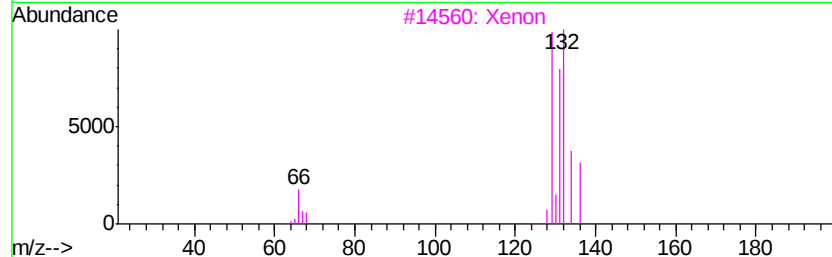
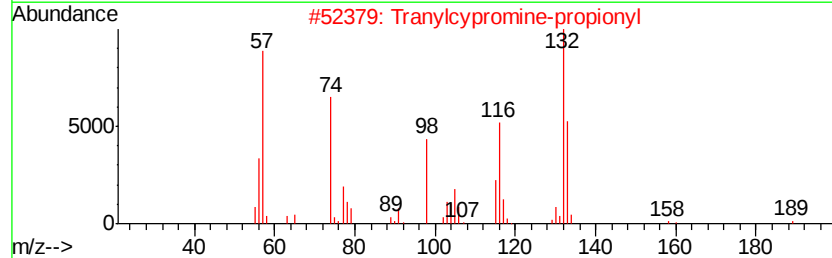
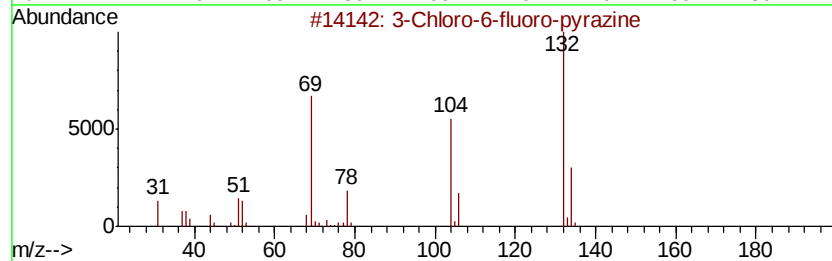
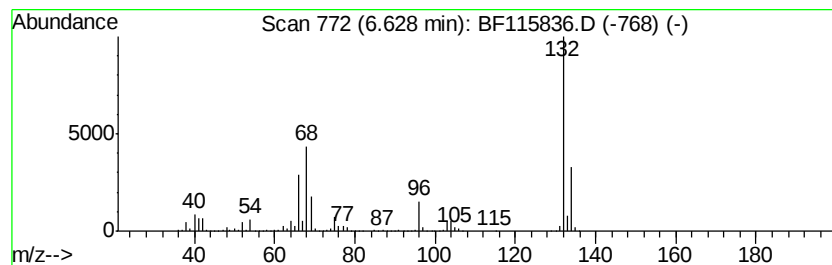
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	76.18 ng	3216990	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Xenon	132	Xe	007440-63-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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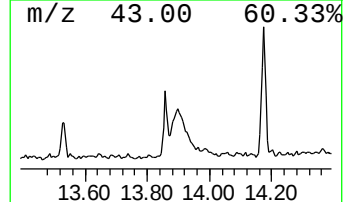
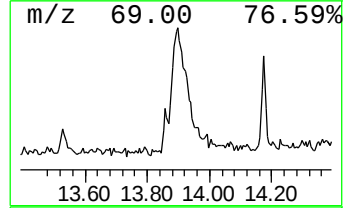
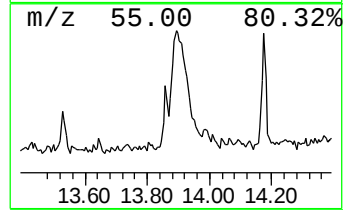
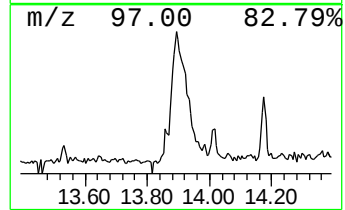
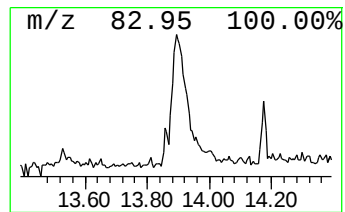
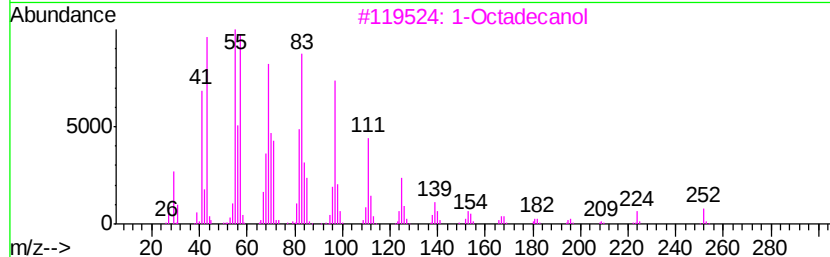
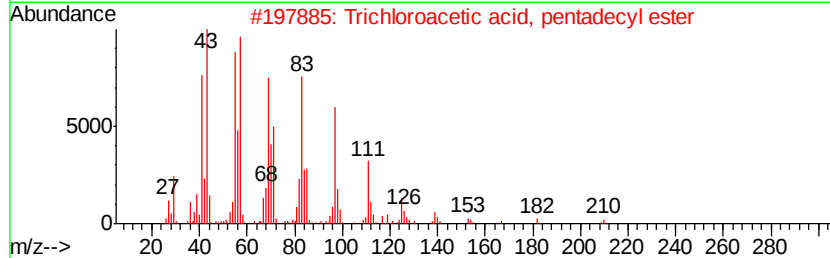
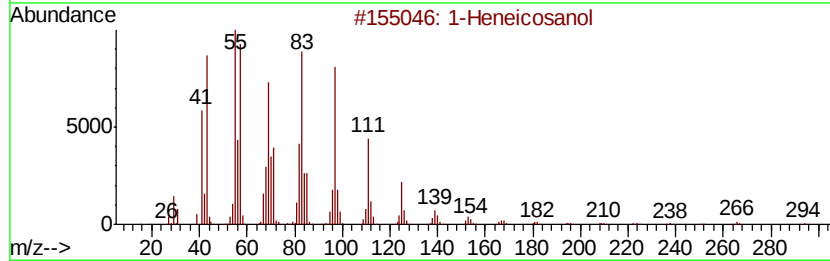
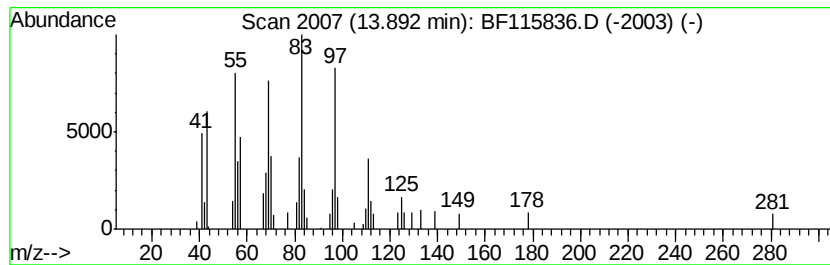
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Peak Number 5 1-Heneicosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.06 ng	175147	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heneicosanol		312 C21H44O	015594-90-8 86
2	Trichloroacetic acid, pentadecyl...		372 C17H31Cl3O2	074339-53-0 58
3	1-Octadecanol		270 C18H38O	000112-92-5 58
4	Thieno[2,3-d]-1,3-thiaselenol-2-...		238 C5H2S3Se	081803-09-0 53
5	1-Nonadecene		266 C19H38	018435-45-5 53



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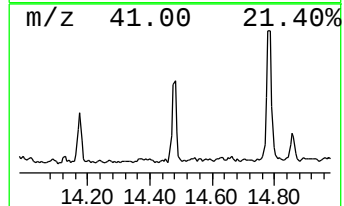
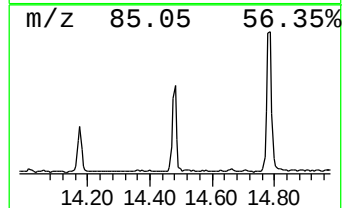
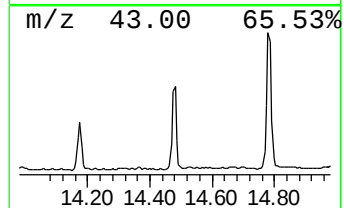
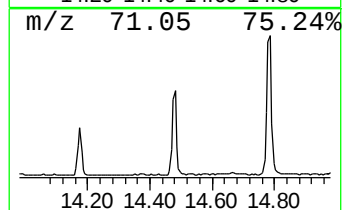
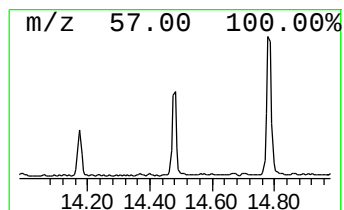
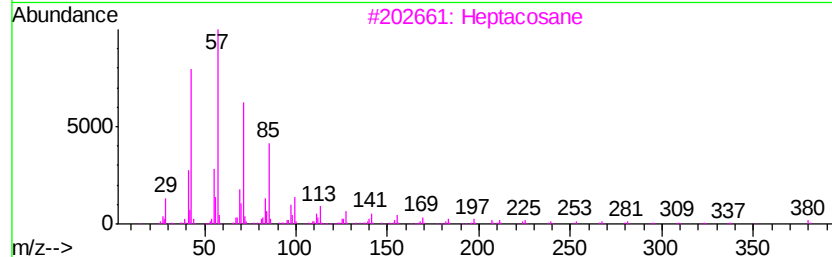
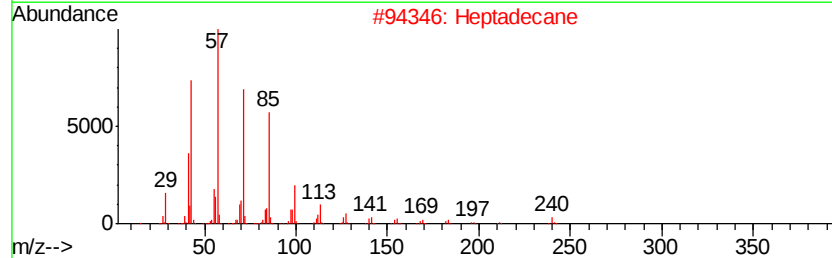
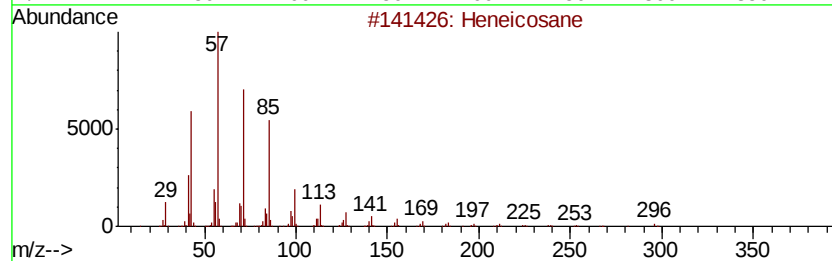
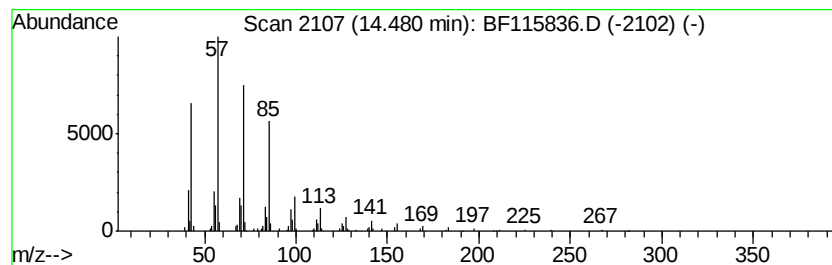
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	3.06 ng	175664	Chrysene-d12	14.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Heptadecane		240	C17H36	000629-78-7	91
3	Heptacosane		380	C27H56	000593-49-7	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Hexadecane		226	C16H34	000544-76-3	90



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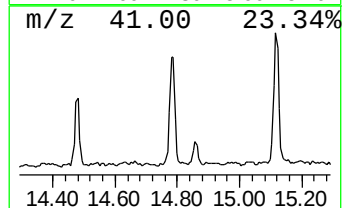
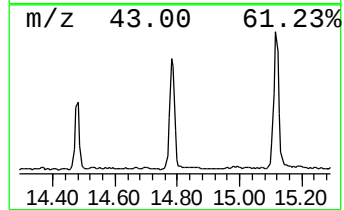
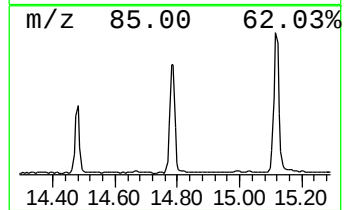
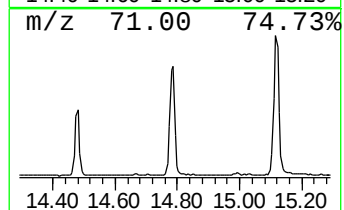
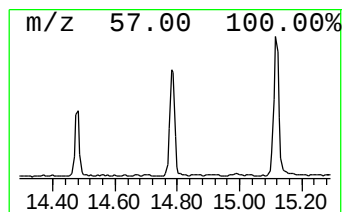
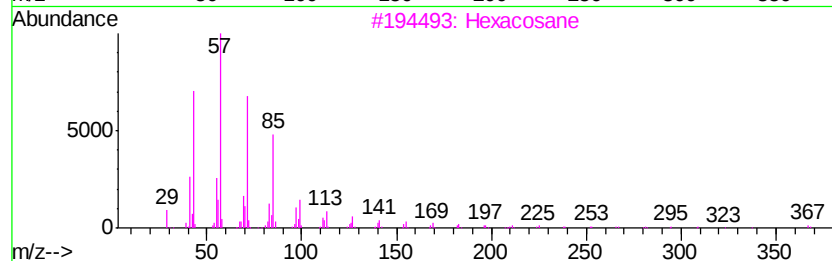
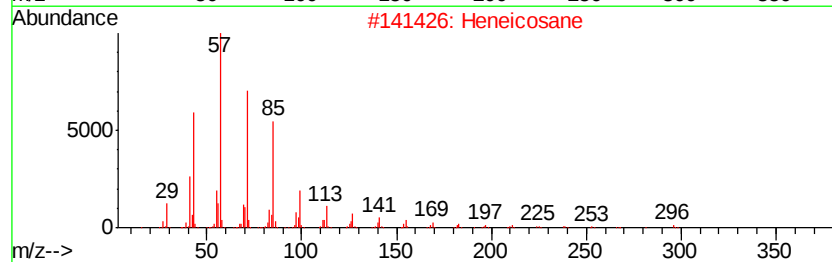
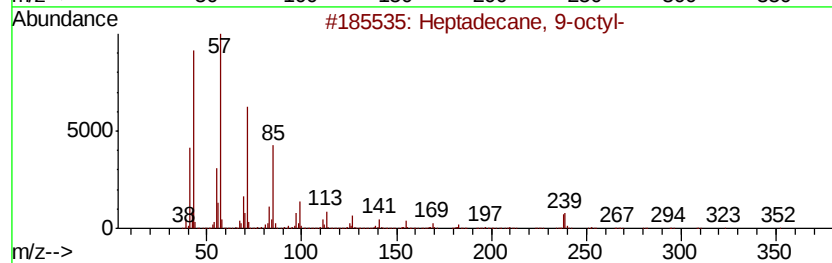
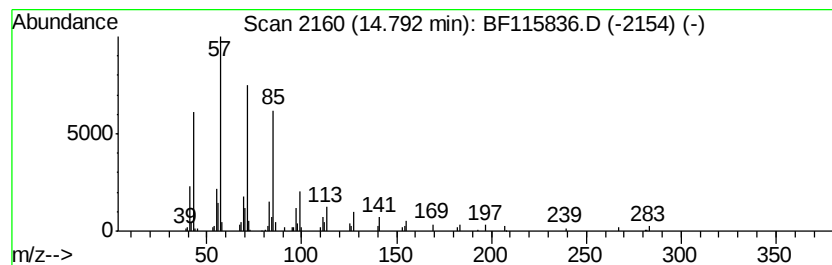
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	4.43 ng	316458	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
Data File : BF115836.D
Acq On : 29 Jul 2019 17:07
Operator : HP/JU
Sample : K4036-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-04

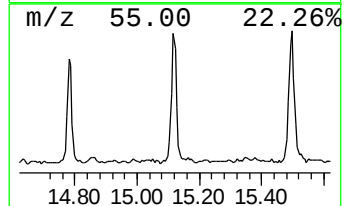
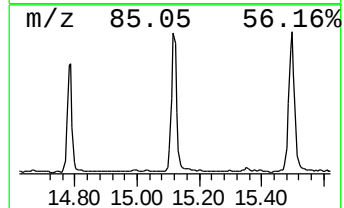
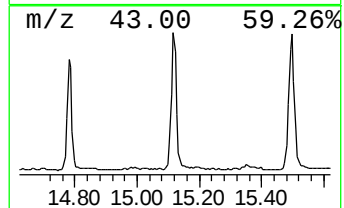
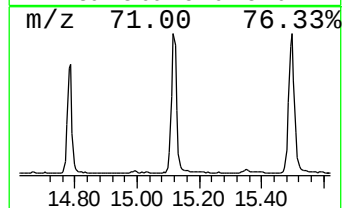
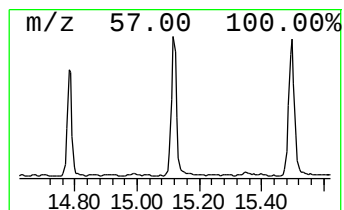
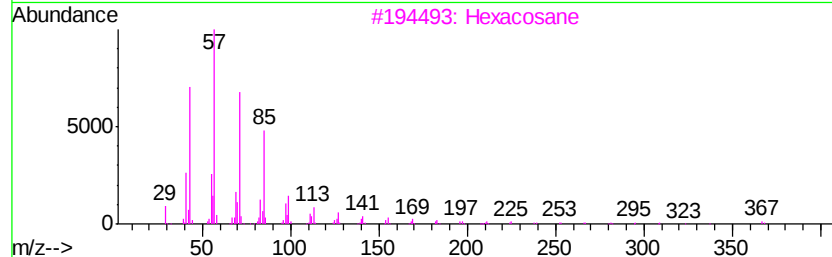
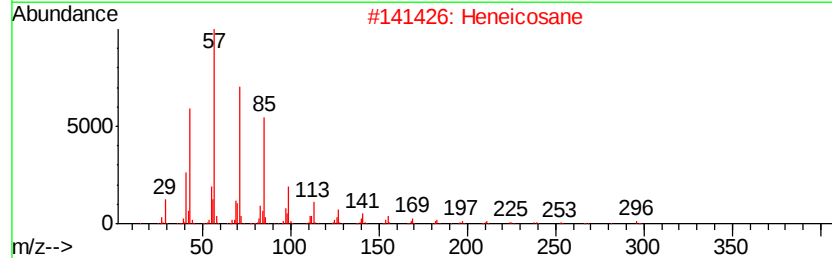
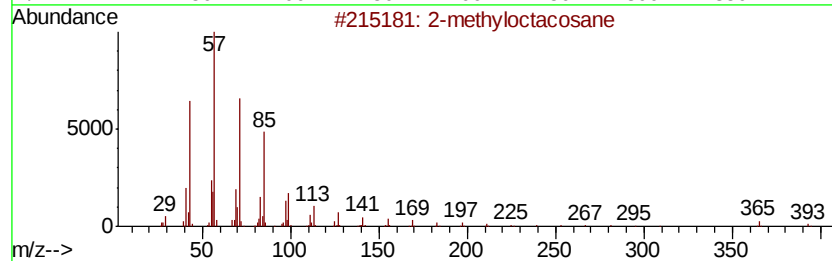
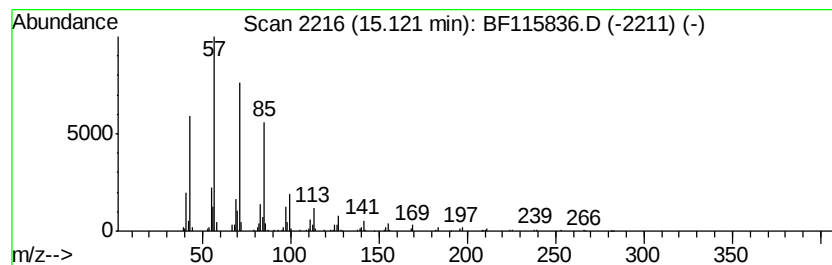
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	6.24 ng	445196	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Octacosane	394	C28H58	000630-02-4	90
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
Data File : BF115836.D
Acq On : 29 Jul 2019 17:07
Operator : HP/JU
Sample : K4036-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

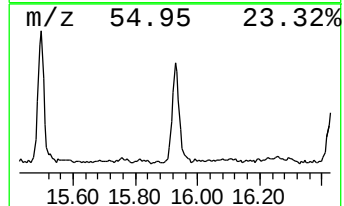
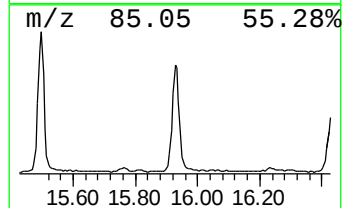
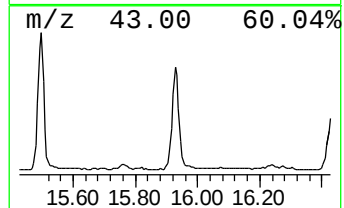
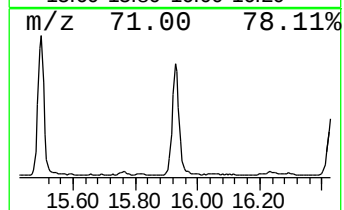
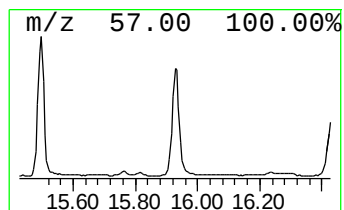
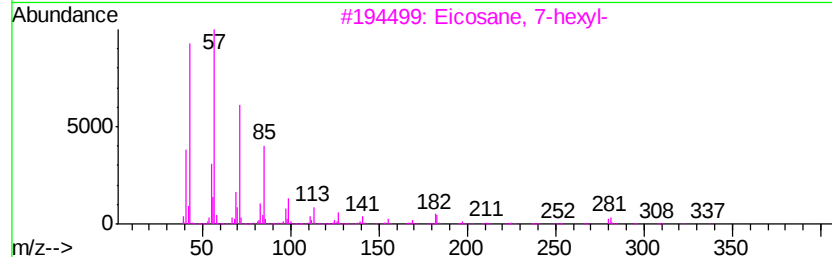
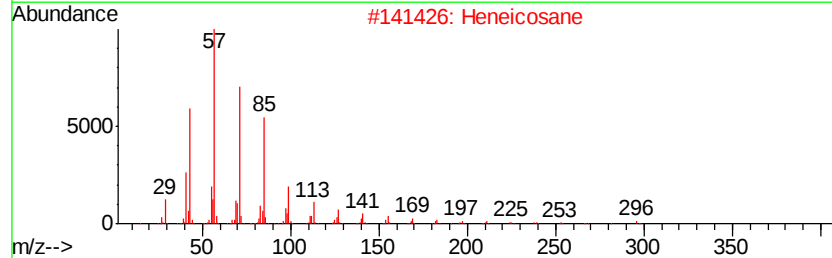
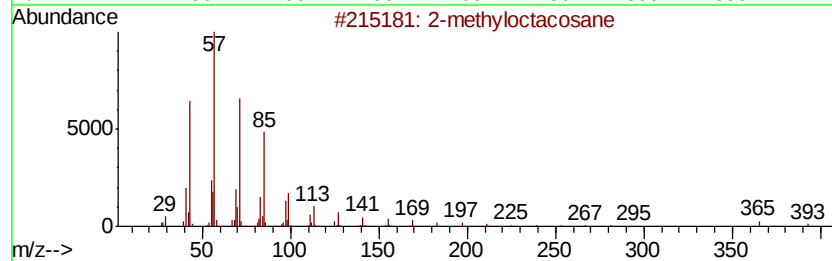
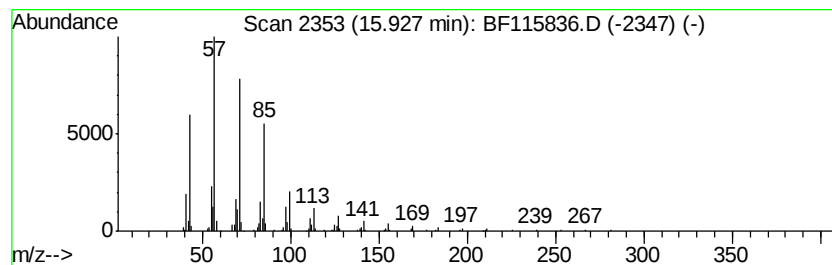
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.93	6.55 ng	467559	Perylene-d12		15.48
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Tetracosane	338	C24H50	000646-31-1	87
5	Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
 Data File : BF115836.D
 Acq On : 29 Jul 2019 17:07
 Operator : HP/JU
 Sample : K4036-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

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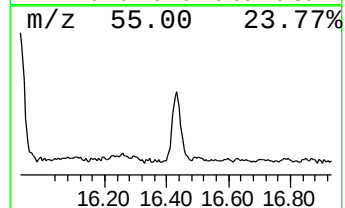
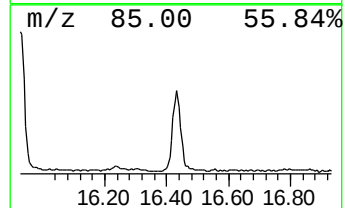
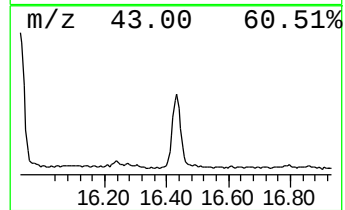
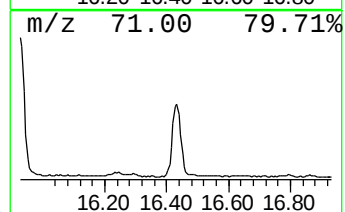
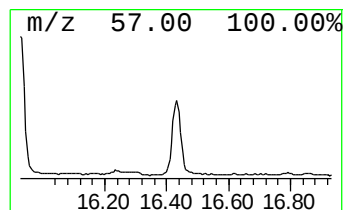
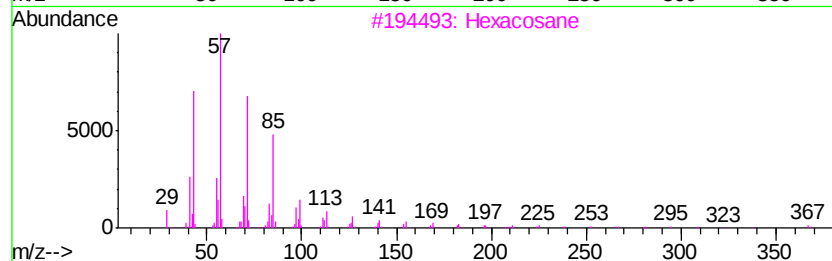
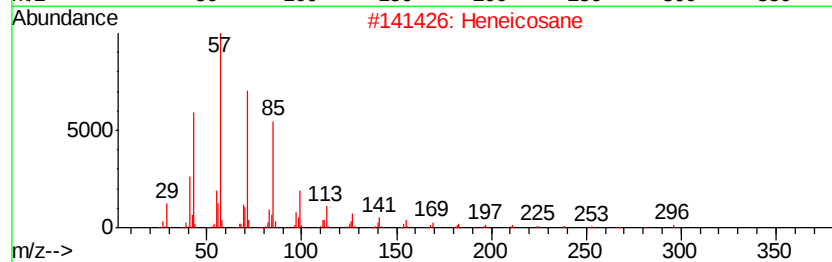
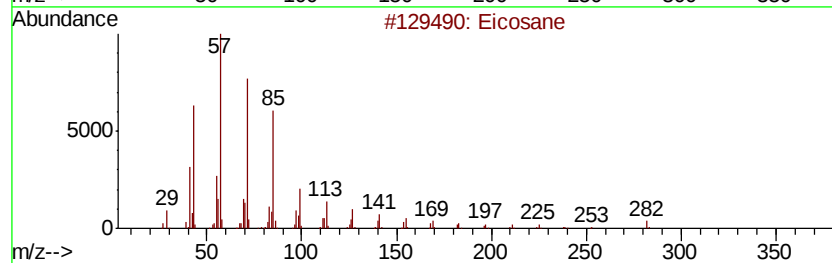
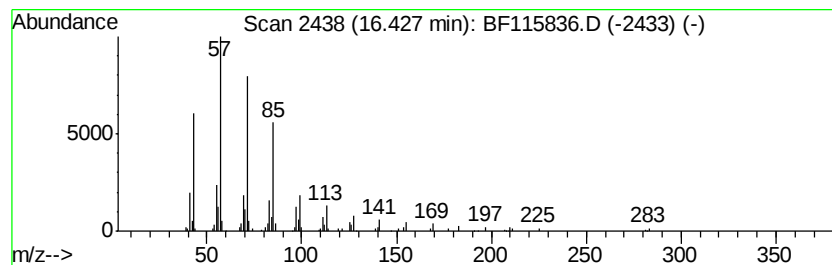
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	4.01 ng	285989	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072919\
Data File : BF115836.D
Acq On : 29 Jul 2019 17:07
Operator : HP/JU
Sample : K4036-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-04

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF071219.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
Butane, 2-methoxy...	2.14	94.3	ng	3980620	1	6.86	844620	20.0
2-Pentanone, 4-hy...	5.07	17.8	ng	750113	1	6.86	844620	20.0
unknown6.63	6.63	76.2	ng	3216990	1	6.86	844620	20.0
1-Heneicosanol	13.89	3.1	ng	175147	5	14.02	1146410	20.0
Heneicosane	14.48	3.1	ng	175664	5	14.02	1146410	20.0
Heptadecane, 9-oc...	14.79	4.4	ng	316458	6	15.48	1427790	20.0
2-methyloctacosane	15.12	6.2	ng	445196	6	15.48	1427790	20.0
Eicosane, 7-hexyl-	15.93	6.5	ng	467559	6	15.48	1427790	20.0
Eicosane	16.43	4.0	ng	285989	6	15.48	1427790	20.0