

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072919\
 Data File : BF115835.D
 Acq On : 29 Jul 2019 16:41
 Operator : HP/JU
 Sample : K4036-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WS-03

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-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	2.134	3	8	38	rVB	2450387	3456808	77.61%	9.228%
2	5.081	502	509	512	rBV	1705999	2116804	47.52%	5.651%
3	5.481	573	577	602	rBV	1871827	1824514	40.96%	4.870%
4	6.486	744	748	765	rBV	1951970	1785536	40.09%	4.766%
5	6.628	768	772	792	rBV	2520524	2648109	59.45%	7.069%
6	6.857	808	811	815	rBV	896109	784143	17.60%	2.093%
7	7.016	834	838	842	rBV	2878965	2626254	58.96%	7.011%
8	7.422	902	907	910	rBV	2338733	2198636	49.36%	5.869%
9	7.775	964	967	978	rVB	65698	61608	1.38%	0.164%
10	8.139	1025	1029	1032	rBV	1107824	979511	21.99%	2.615%
11	8.163	1032	1033	1042	rVB	56961	50128	1.13%	0.134%
12	8.622	1108	1111	1117	rBV	151355	134571	3.02%	0.359%
13	9.151	1197	1201	1207	rBV	47346	71349	1.60%	0.190%
14	9.216	1207	1212	1215	rBV	4262164	3907131	87.72%	10.430%
15	9.604	1275	1278	1287	rVB	78199	84351	1.89%	0.225%
16	9.892	1323	1327	1339	rVB	1412219	1190209	26.72%	3.177%
17	10.504	1426	1431	1434	rBV2	47476	59668	1.34%	0.159%
18	10.680	1457	1461	1469	rBV	681131	674188	15.14%	1.800%
19	11.333	1568	1572	1574	rBV	82341	75023	1.68%	0.200%
20	11.374	1574	1579	1587	rVB	1283060	1289081	28.94%	3.441%
21	12.127	1703	1707	1711	rBV	52190	46342	1.04%	0.124%
22	12.680	1795	1801	1814	rBV4	38706	96658	2.17%	0.258%
23	12.963	1844	1849	1852	rBV	4436606	4454104	100.00%	11.890%
24	13.651	1963	1966	1970	rBV2	48080	45222	1.02%	0.121%
25	13.857	1998	2001	2004	rBV	98697	85326	1.92%	0.228%
26	13.898	2004	2008	2020	rVV5	45899	138654	3.11%	0.370%
27	14.015	2024	2028	2038	rVB	1219917	1178544	26.46%	3.146%
28	14.174	2051	2055	2059	rBV	192419	167592	3.76%	0.447%
29	14.480	2102	2107	2111	rBV	355050	351033	7.88%	0.937%
30	14.780	2154	2158	2166	rBV	540339	587584	13.19%	1.569%
31	15.121	2211	2216	2223	rBV	633132	754504	16.94%	2.014%
32	15.480	2271	2277	2290	rBV2	898124	1894280	42.53%	5.057%
33	15.927	2347	2353	2367	rBV	531511	844499	18.96%	2.254%
34	16.433	2432	2439	2454	rBV	293747	557726	12.52%	1.489%

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

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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.021	2532	2539	2547	rBV2	84270	180283	4.05%	0.481%
36	17.715	2653	2657	2666	rVB2	28861	60542	1.36%	0.162%

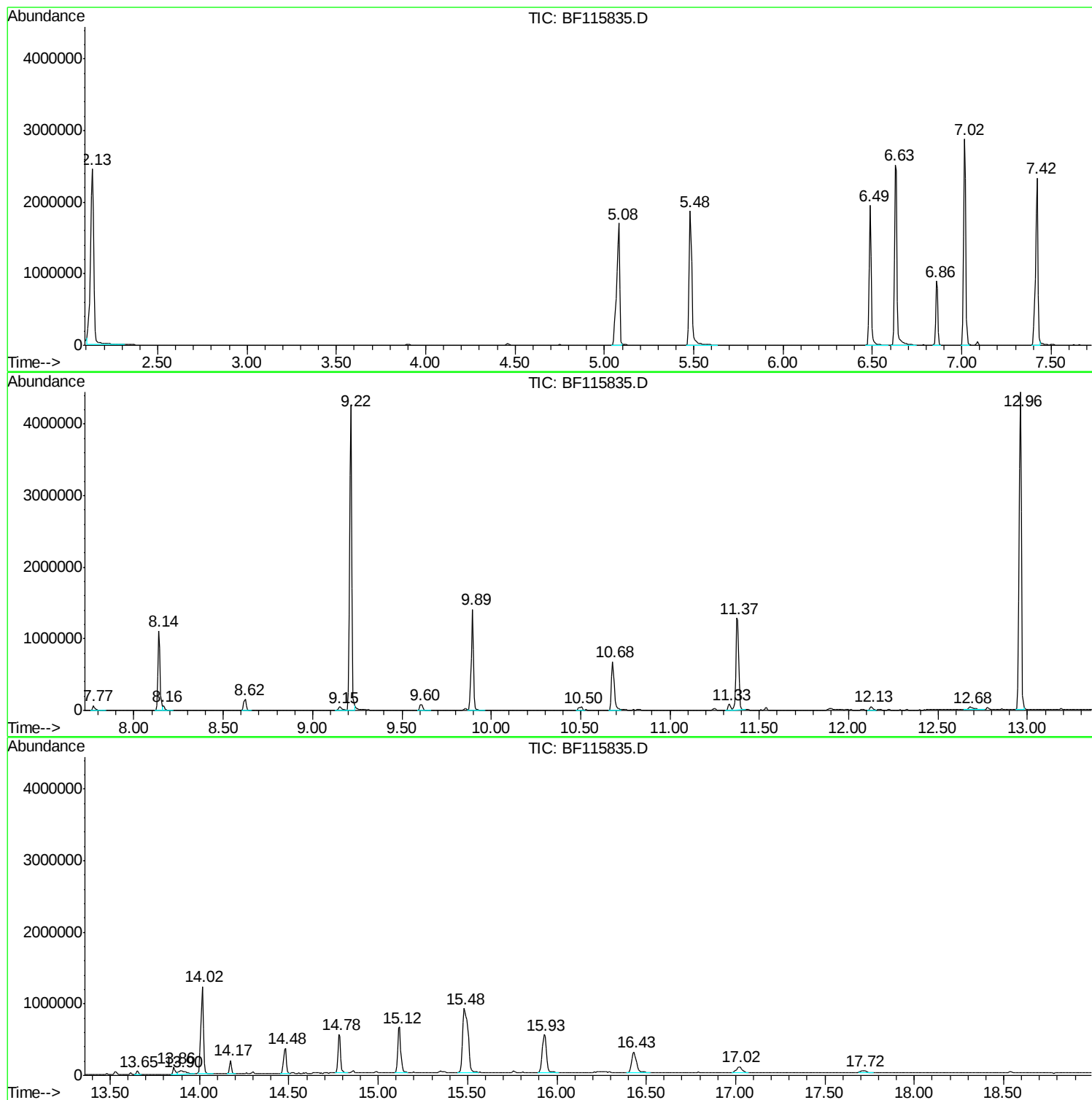
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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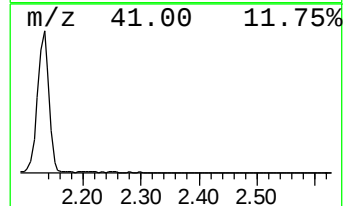
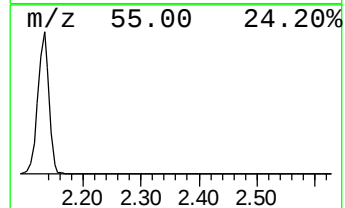
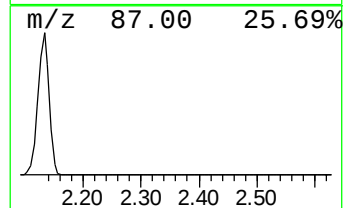
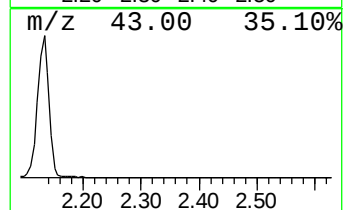
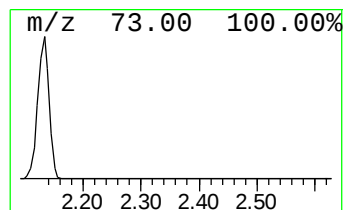
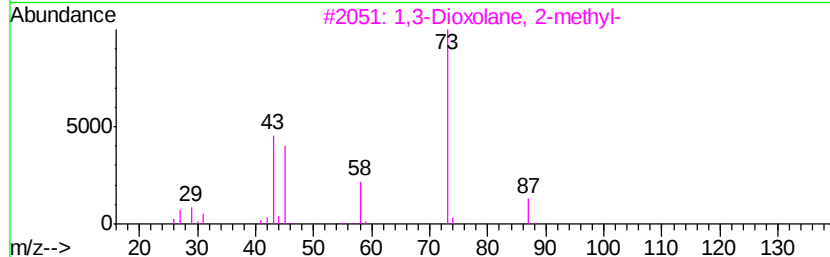
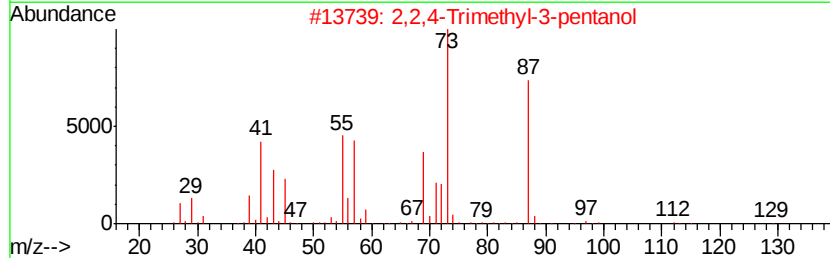
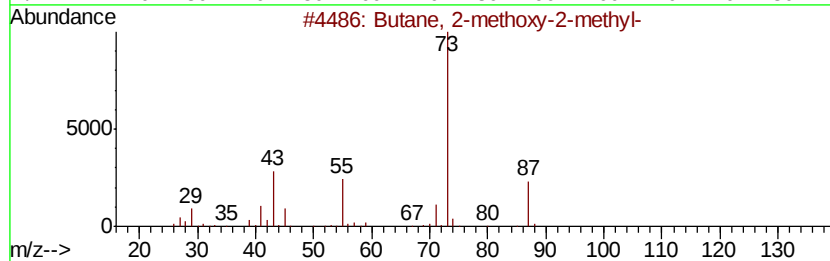
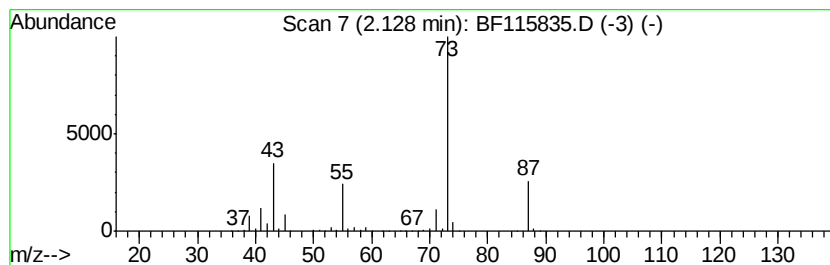
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	88.17 ng	3456810	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	37
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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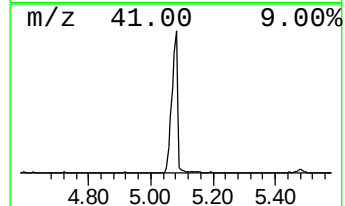
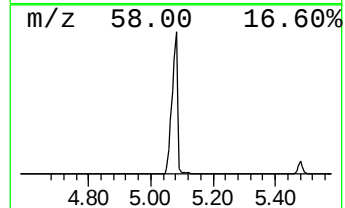
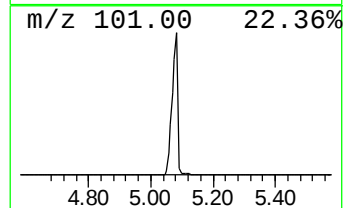
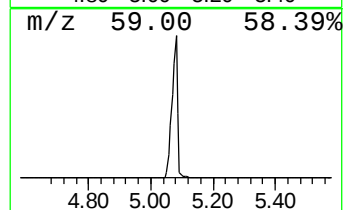
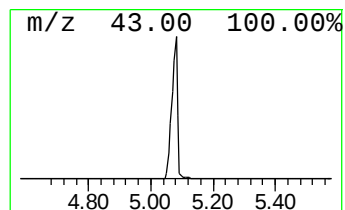
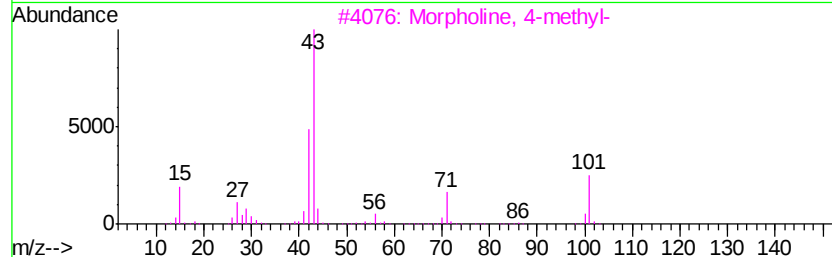
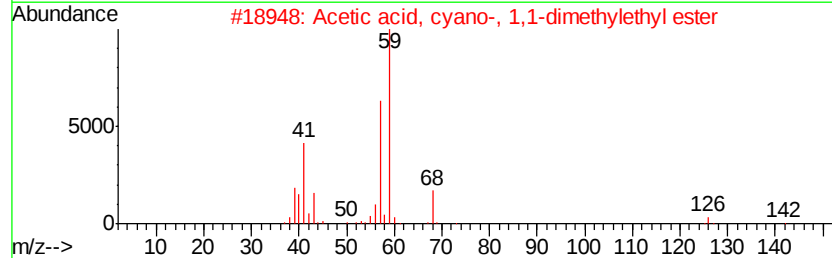
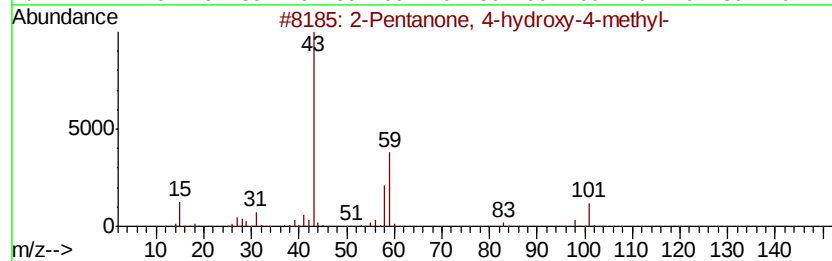
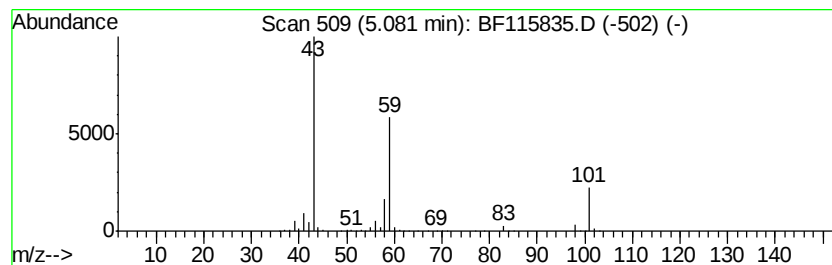
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	53.99 ng	2116800	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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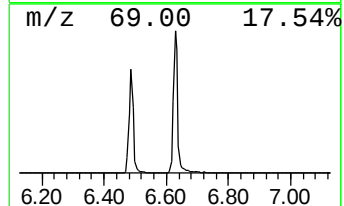
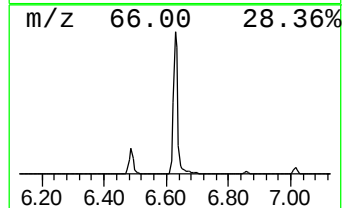
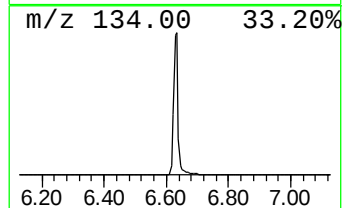
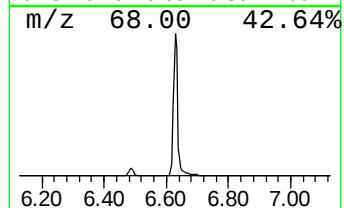
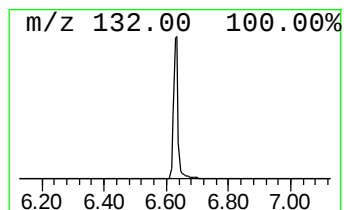
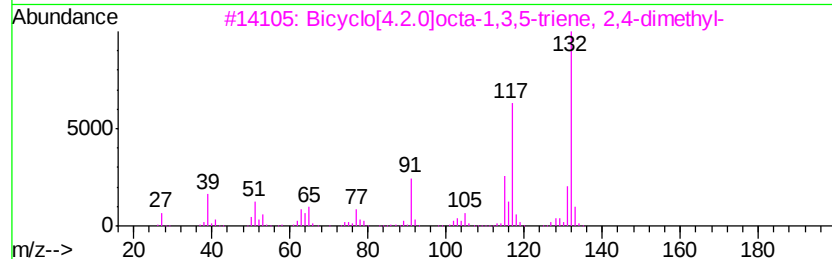
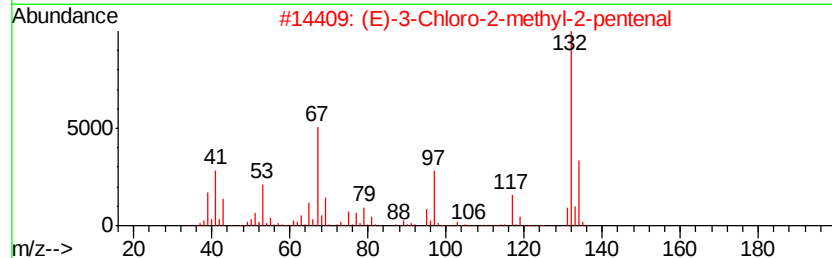
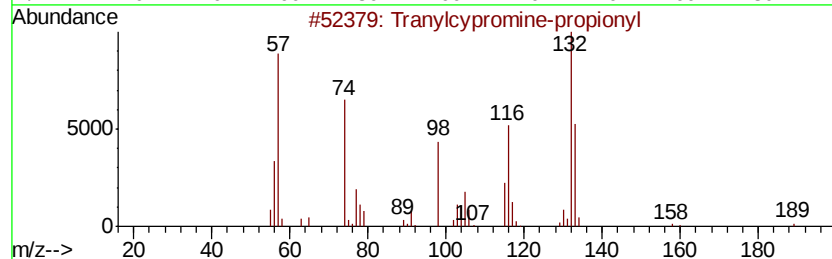
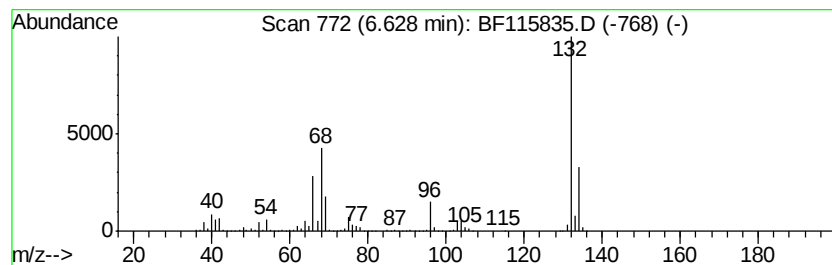
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	67.54 ng	2648110	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcyppromine-propionyl	189	C12H15NO	1000123-86-3	10
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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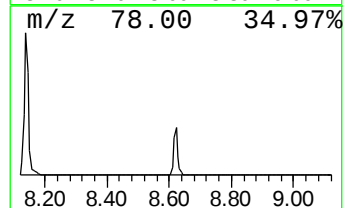
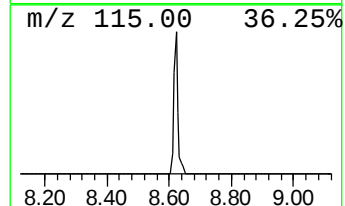
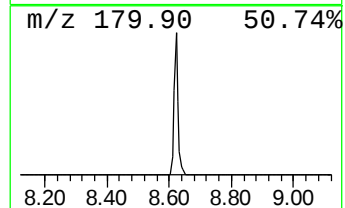
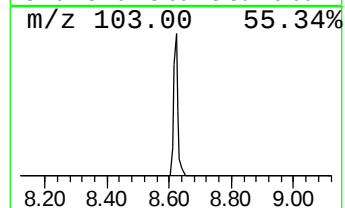
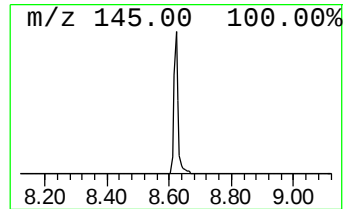
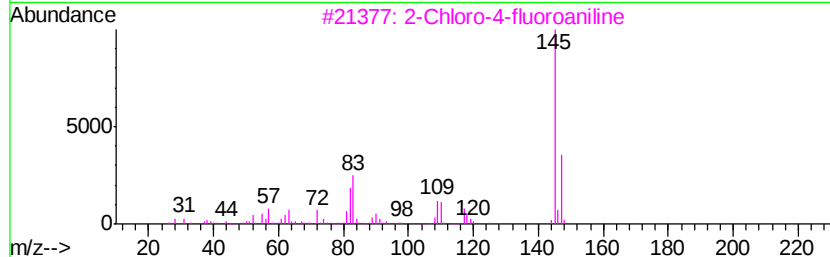
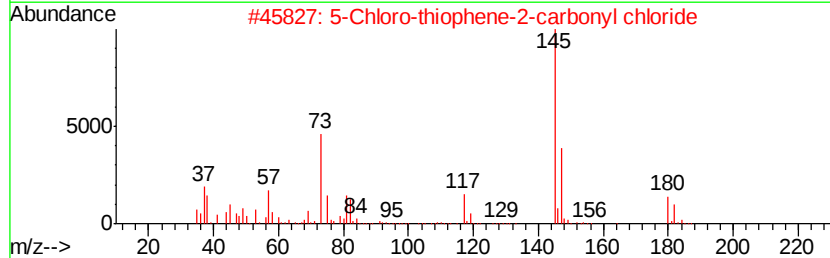
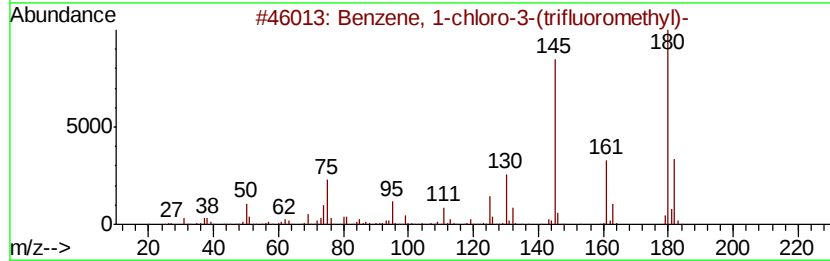
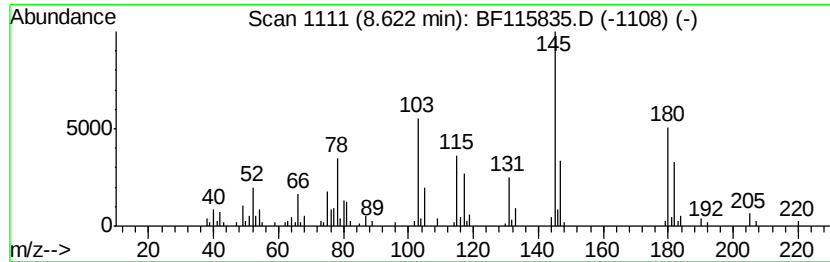
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown8.62 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	2.75 ng	134571	Naphthalene-d8	8.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-chloro-3-(trifluorome...	180	C7H4ClF3	000098-15-7	22
2		5-Chloro-thiophene-2-carbonyl ch...	180	C5H2Cl2OS	1000296-93-2	16
3		2-Chloro-4-fluoroaniline	145	C6H5ClFN	002106-02-7	14
4		7-Quinolinol	145	C9H7NO	000580-20-1	14
5		4-Ethyl-1,2,4-triazol-3-thione-5...	145	C4H7N3OS	053249-23-3	14



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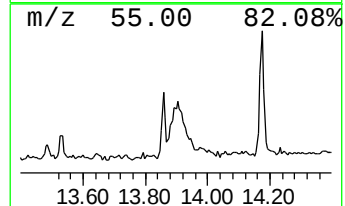
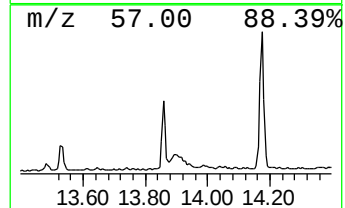
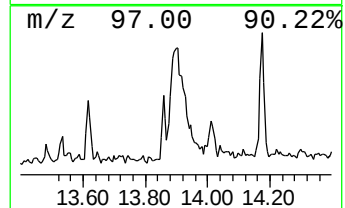
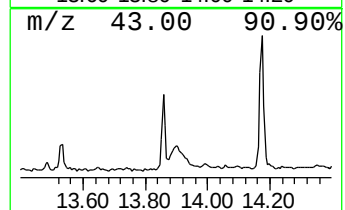
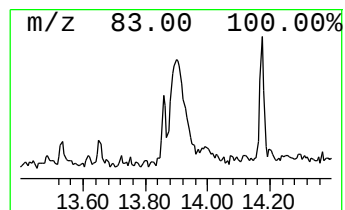
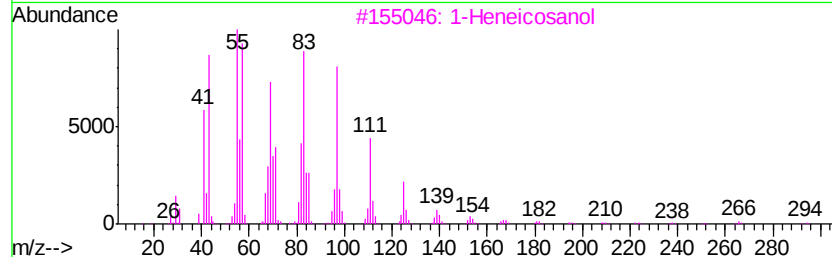
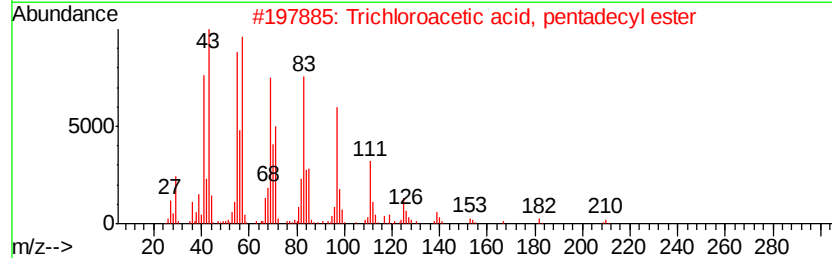
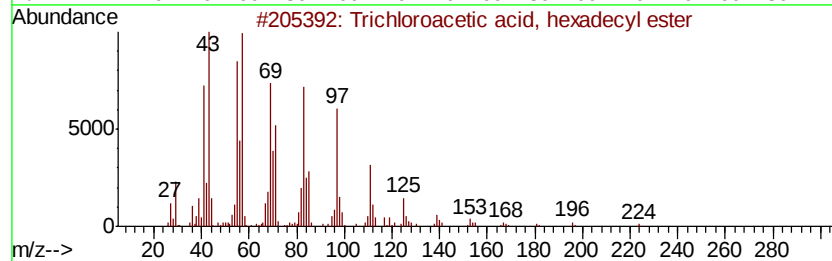
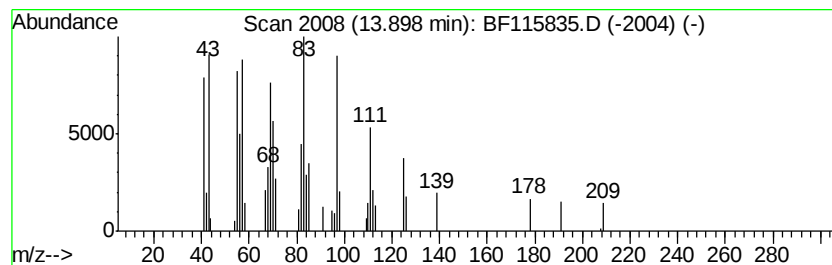
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	2.35 ng	138654	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
3		1-Heneicosanol	312	C21H44O	015594-90-8	90
4		1-Heptacosanol	396	C27H56O	002004-39-9	90
5		1-Nonadecene	266	C19H38	018435-45-5	90



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Data File : BF115835.D
Acq On : 29 Jul 2019 16:41
Operator : HP/JU
Sample : K4036-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WS-03

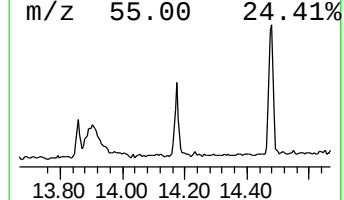
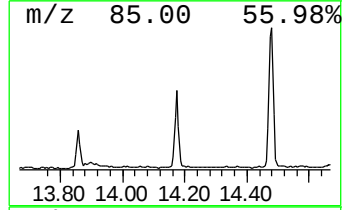
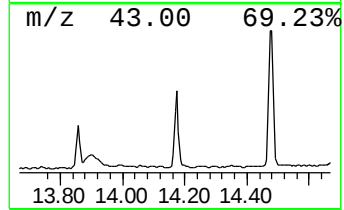
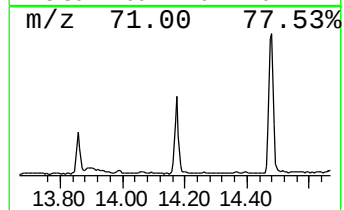
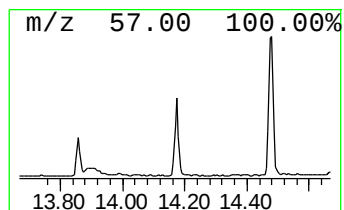
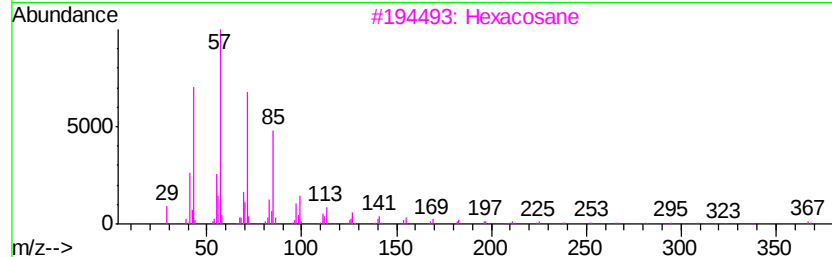
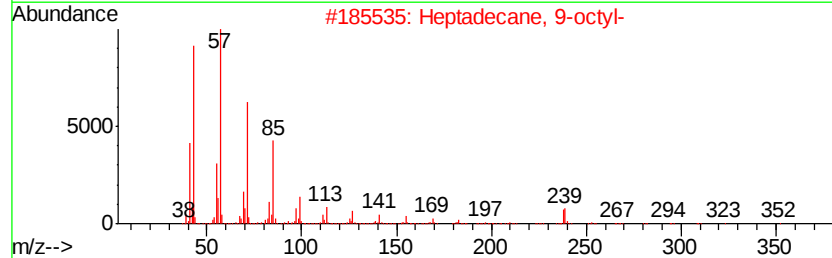
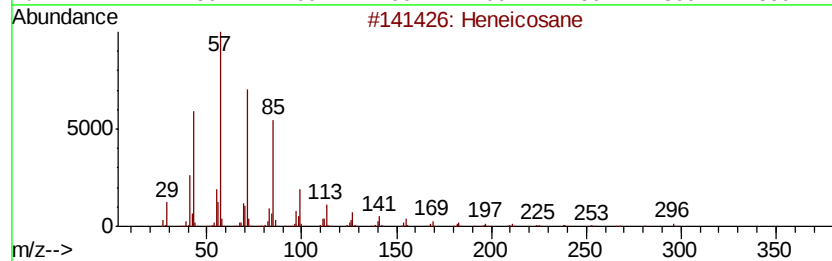
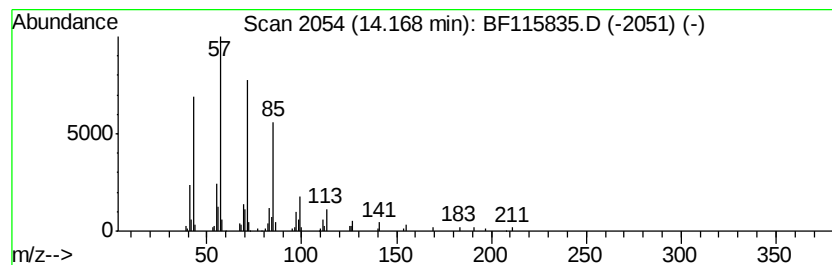
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	2.84 ng	167592	Chrysene-d12	14.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Hexadecane	226	C16H34	000544-76-3	86
5		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
Data File : BF115835.D
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Operator : HP/JU
Sample : K4036-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

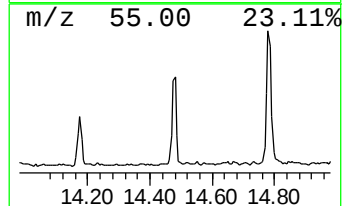
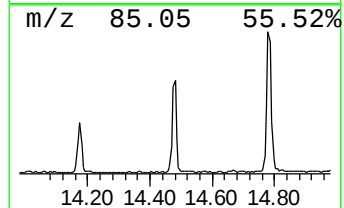
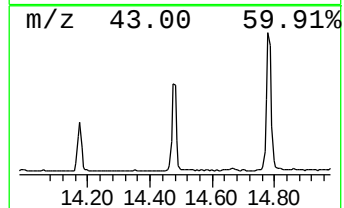
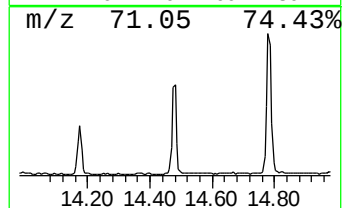
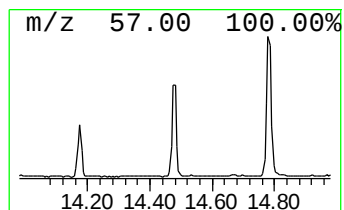
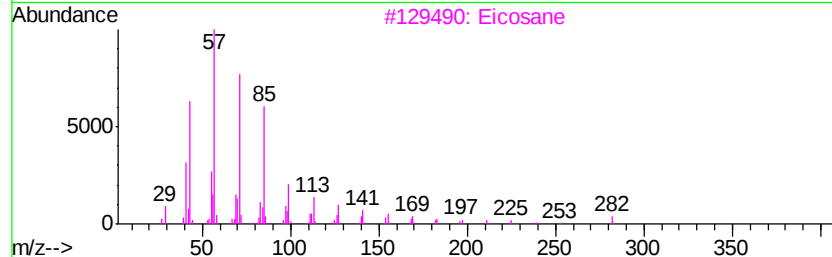
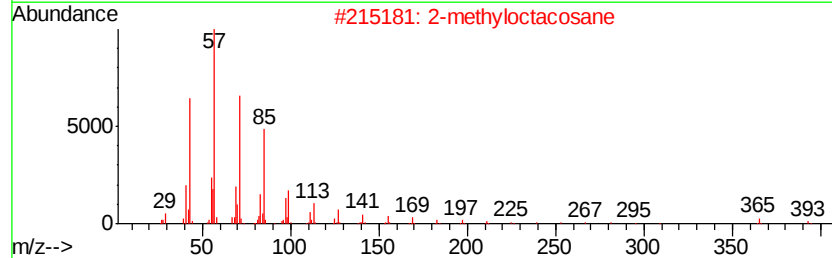
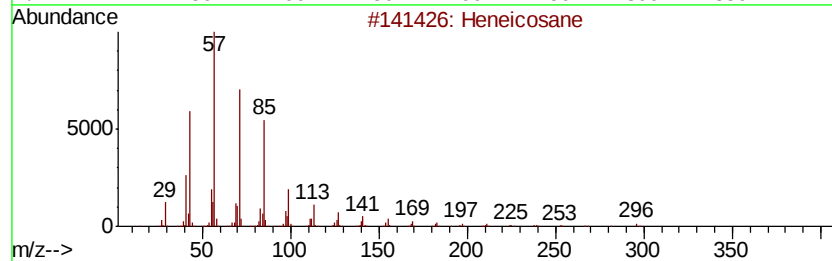
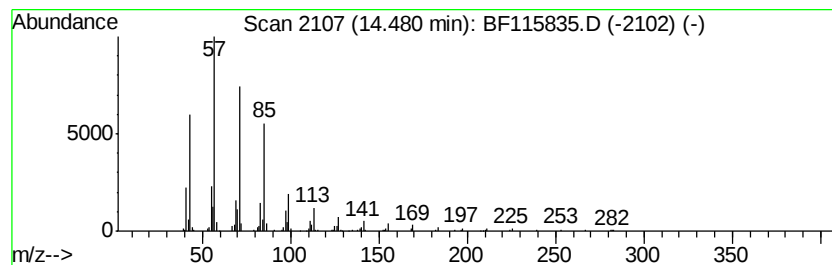
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.48	5.96 ng	351033	Chrysene-d12	14.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	2-methyloctacosane	408 C29H60	1000376-72-8	91
3	Eicosane	282 C20H42	000112-95-8	91
4	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91
5	Octacosane	394 C28H58	000630-02-4	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
Data File : BF115835.D
Acq On : 29 Jul 2019 16:41
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Sample : K4036-03
Misc :
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Instrument :
BNA_F
ClientSampleId :
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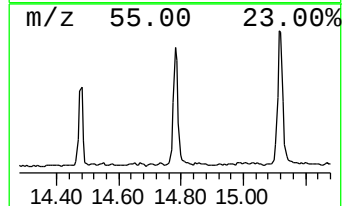
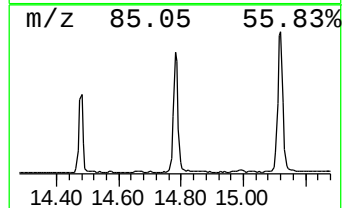
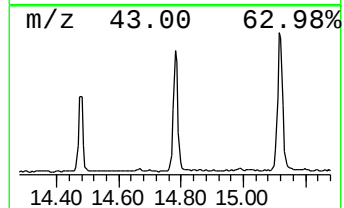
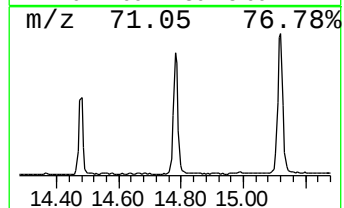
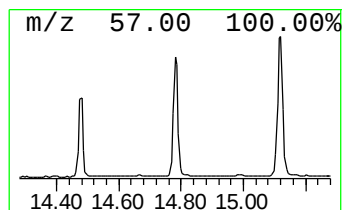
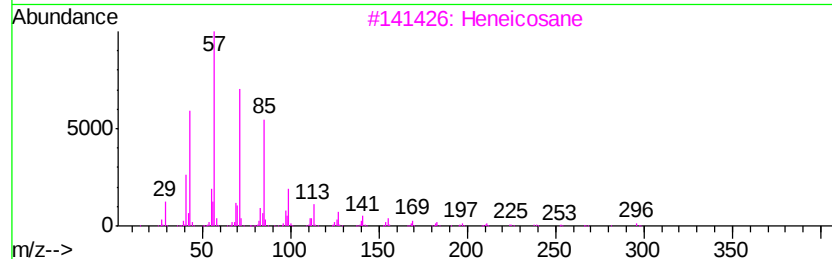
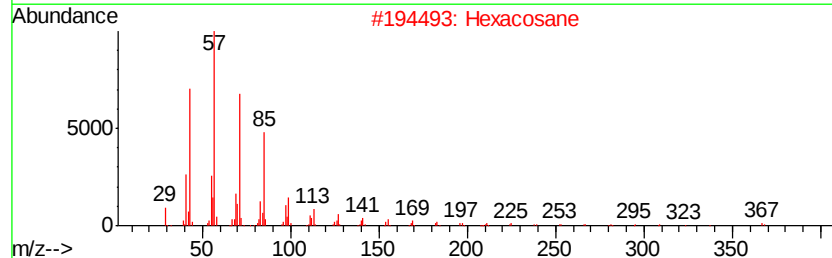
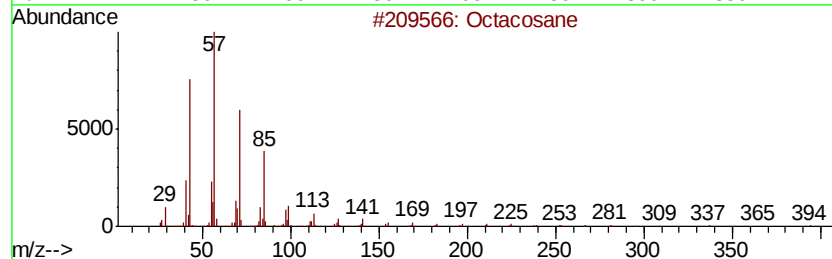
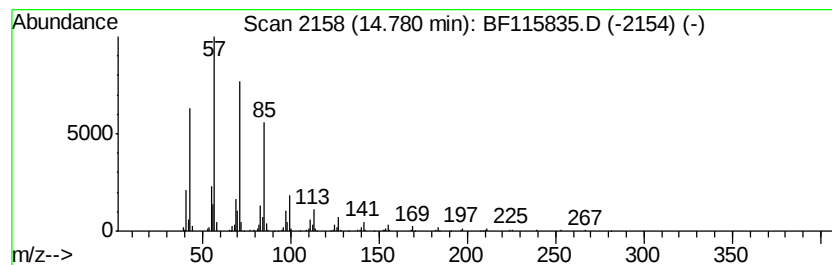
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	6.20 ng	587584	Perylene-d12	15.48

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		Heneicosane	296	C21H44	000629-94-7	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Hexadecane	226	C16H34	000544-76-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
Data File : BF115835.D
Acq On : 29 Jul 2019 16:41
Operator : HP/JU
Sample : K4036-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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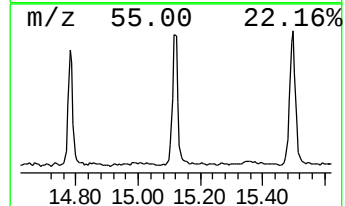
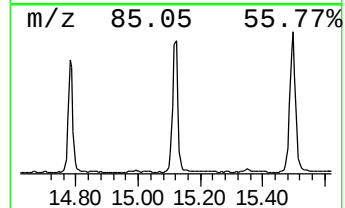
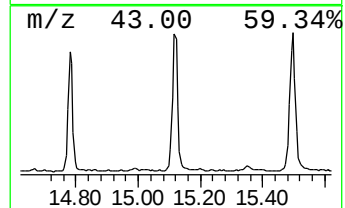
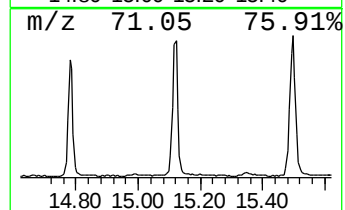
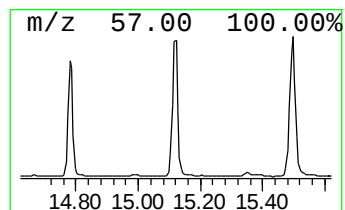
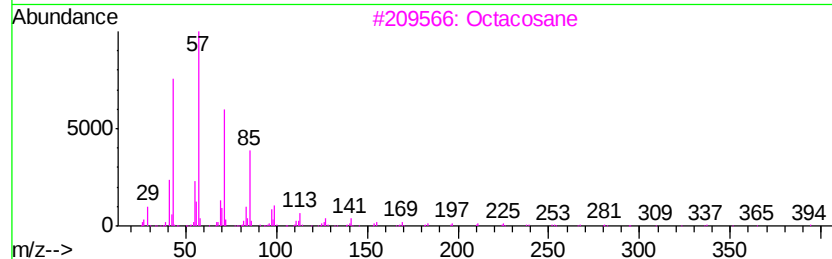
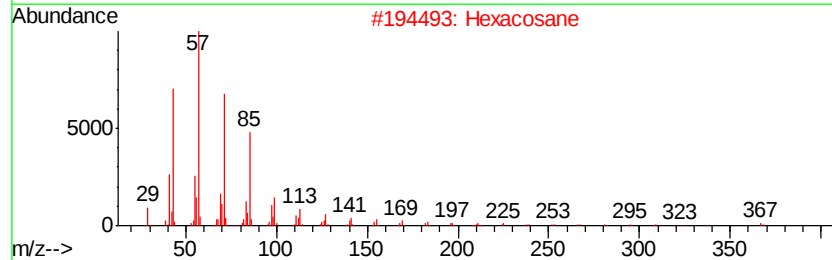
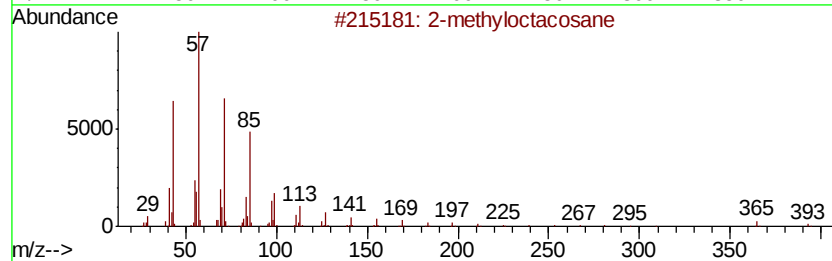
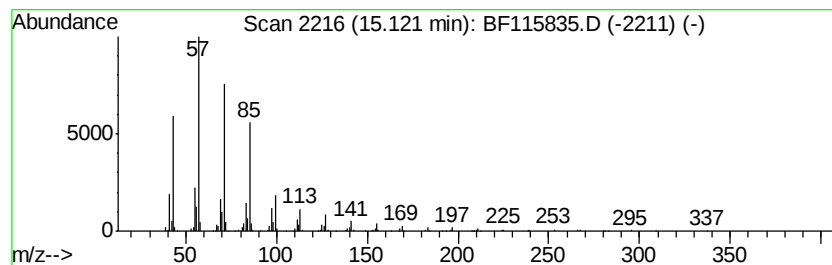
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	7.97 ng	754504	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
Data File : BF115835.D
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ClientSampleId :
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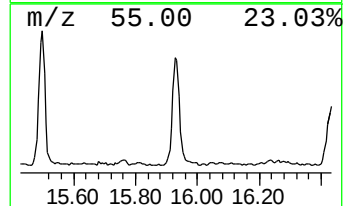
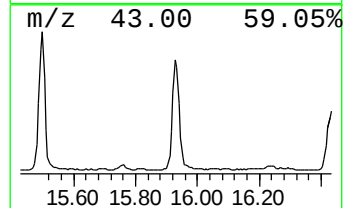
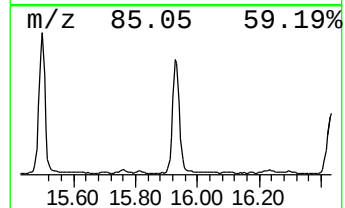
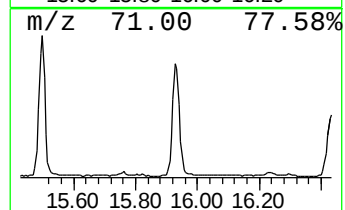
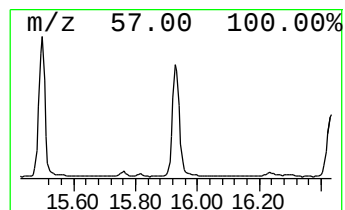
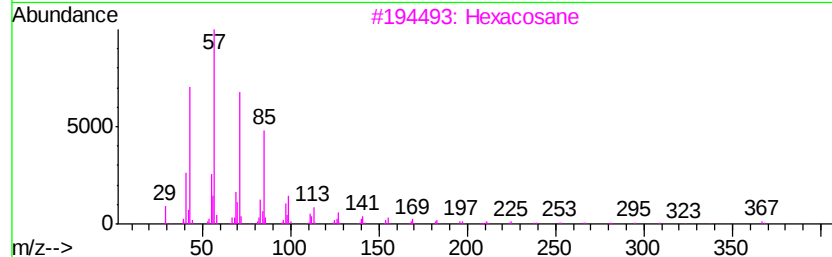
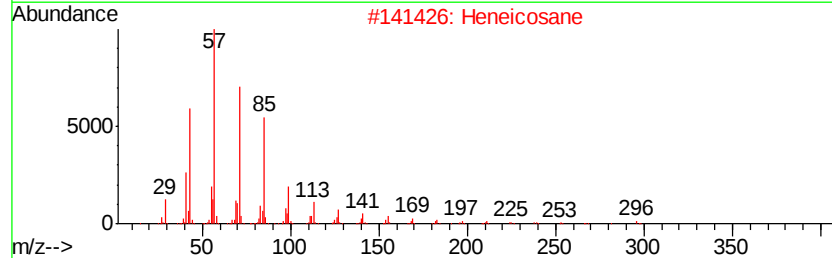
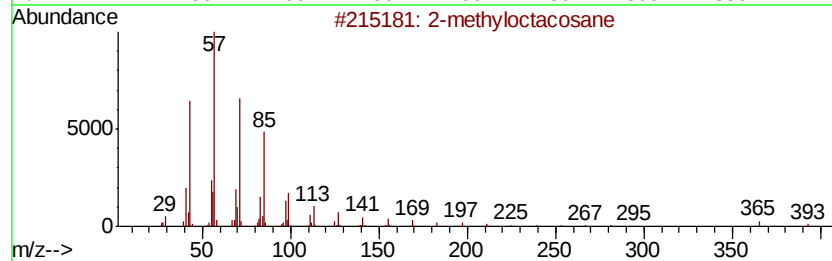
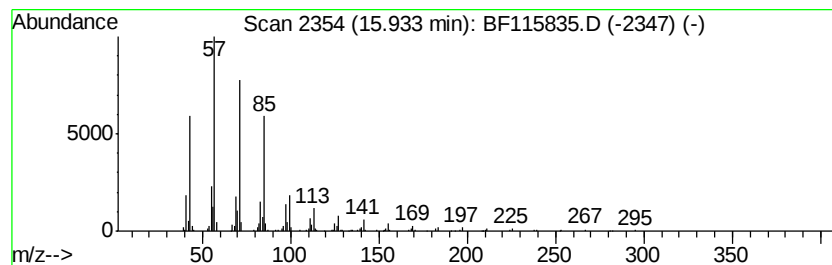
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	8.92 ng	844499	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	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Pentacosane	352	C25H52	000629-99-2	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072919\
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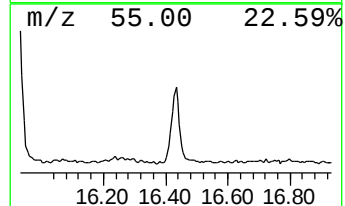
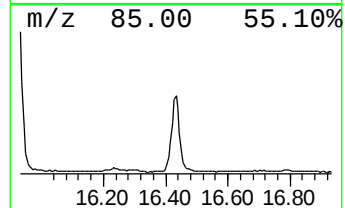
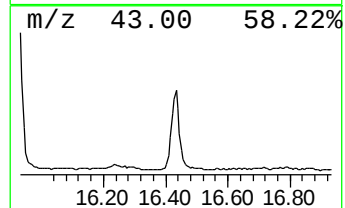
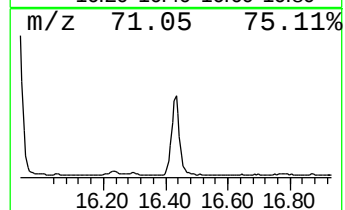
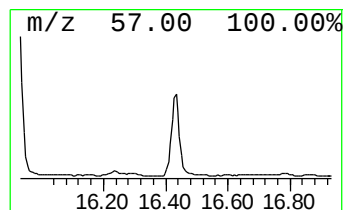
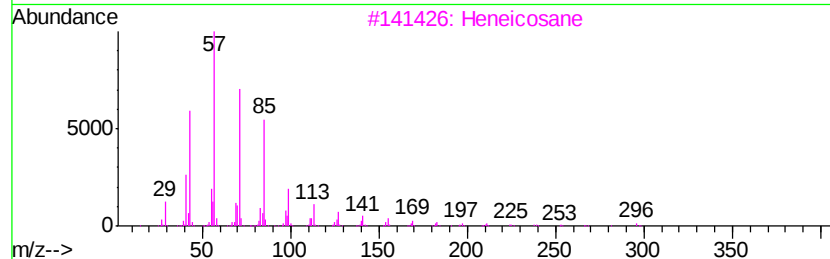
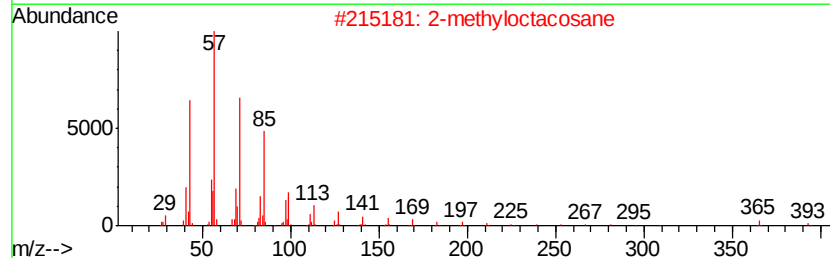
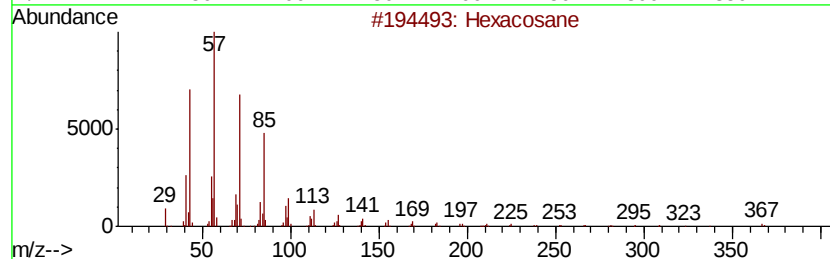
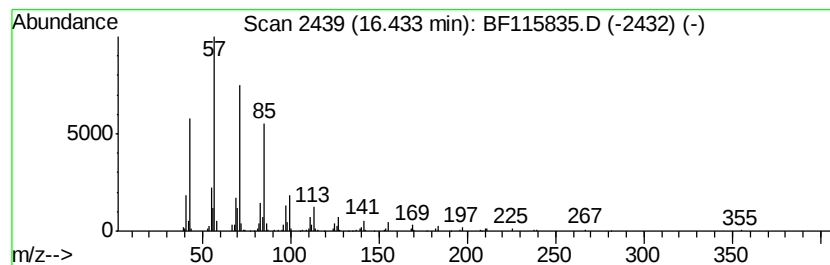
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	5.89 ng	557726	Perylene-d12	15.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexacosane	366 C26H54	000630-01-3	91
2	2-methyloctacosane	408 C29H60	1000376-72-8	91
3	Heneicosane	296 C21H44	000629-94-7	91
4	Tetracosane	338 C24H50	000646-31-1	91
5	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072919\
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Sample : K4036-03
Misc :
ALS Vial : 5 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	54.0	ng	2116800	1	6.86	784143	20.0
unknown6.63	6.63	67.5	ng	2648110	1	6.86	784143	20.0
unknown8.62	8.62	2.8	ng	134571	2	8.14	979511	20.0
Trichloroacetic a...	13.90	2.4	ng	138654	5	14.02	1178540	20.0
Heneicosane	14.17	2.8	ng	167592	5	14.02	1178540	20.0
Eicosane	14.48	6.0	ng	351033	5	14.02	1178540	20.0
Octacosane	14.78	6.2	ng	587584	6	15.48	1894280	20.0
2-methyloctacosane	15.12	8.0	ng	754504	6	15.48	1894280	20.0
Heptadecane, 9-oc...	15.93	8.9	ng	844499	6	15.48	1894280	20.0
Hexacosane	16.43	5.9	ng	557726	6	15.48	1894280	20.0