

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112519\
 Data File : BF117992.D
 Acq On : 26 Nov 2019 3:36
 Operator : JU
 Sample : K5839-01 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHIPPS-BH-NW-01

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-BF111319.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	8	13	23	rVB	246542	313767	22.50%	1.839%
2	3.969	315	320	327	rBV	18378	24670	1.77%	0.145%
3	5.092	507	511	523	rVB	226770	231310	16.59%	1.355%
4	5.498	576	580	584	rBV	1408024	1168098	83.76%	6.845%
5	6.510	748	752	759	rBV	1656477	1388413	99.56%	8.136%
6	6.604	765	768	773	rVB	40464	27911	2.00%	0.164%
7	6.657	773	777	780	rBV	1694483	1394538	100.00%	8.172%
8	6.892	813	817	820	rBV	1210381	1048583	75.19%	6.145%
9	7.045	839	843	847	rBV	1163956	967799	69.40%	5.671%
10	7.451	908	912	915	rBV	849872	687673	49.31%	4.030%
11	7.486	915	918	922	rVB2	21017	22666	1.63%	0.133%
12	8.181	1029	1036	1039	rBV	1359637	1155858	82.88%	6.773%
13	8.239	1043	1046	1049	rVB	32538	29005	2.08%	0.170%
14	8.469	1081	1085	1090	rBV5	18981	23210	1.66%	0.136%
15	8.598	1104	1107	1109	rBV	44322	35023	2.51%	0.205%
16	8.769	1133	1136	1140	rVB	70849	52536	3.77%	0.308%
17	9.204	1207	1210	1213	rVB	43554	40201	2.88%	0.236%
18	9.257	1215	1219	1222	rBV	1679005	1381774	99.08%	8.097%
19	9.333	1229	1232	1236	rBV	63226	61105	4.38%	0.358%
20	9.651	1283	1286	1290	rBV	171302	167940	12.04%	0.984%
21	9.869	1318	1323	1328	rBV2	30971	31021	2.22%	0.182%
22	9.939	1331	1335	1339	rBV	1360979	1139862	81.74%	6.680%
23	10.727	1466	1469	1481	rVB	791992	686081	49.20%	4.020%
24	10.833	1484	1487	1494	rVB	52986	54858	3.93%	0.321%
25	11.433	1585	1589	1592	rBV	1153924	947429	67.94%	5.552%
26	11.957	1674	1678	1691	rVB	281379	287846	20.64%	1.687%
27	12.645	1792	1795	1797	rBV	87347	92389	6.63%	0.541%
28	12.663	1797	1798	1808	rVB2	106419	125578	9.00%	0.736%
29	12.745	1808	1812	1818	rBV	109025	124825	8.95%	0.731%
30	12.880	1832	1835	1842	rVB2	25228	29282	2.10%	0.172%
31	13.021	1855	1859	1862	rBV	1218724	997907	71.56%	5.848%
32	13.251	1896	1898	1901	rBV4	15783	16467	1.18%	0.096%
33	13.927	2010	2013	2019	rBV3	80967	135431	9.71%	0.794%
34	14.080	2035	2039	2043	rBV	863217	785487	56.33%	4.603%

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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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.239	2064	2066	2069	rVB	44995	43735	3.14%	0.256%
36	14.545	2116	2118	2121	rBV	69298	65075	4.67%	0.381%
37	14.862	2169	2172	2176	rVB	112919	108477	7.78%	0.636%
38	15.215	2229	2232	2235	rBV	109087	112620	8.08%	0.660%
39	15.586	2290	2295	2309	rVB	568108	942303	67.57%	5.522%
40	16.062	2373	2376	2380	rVB	84288	116297	8.34%	0.681%

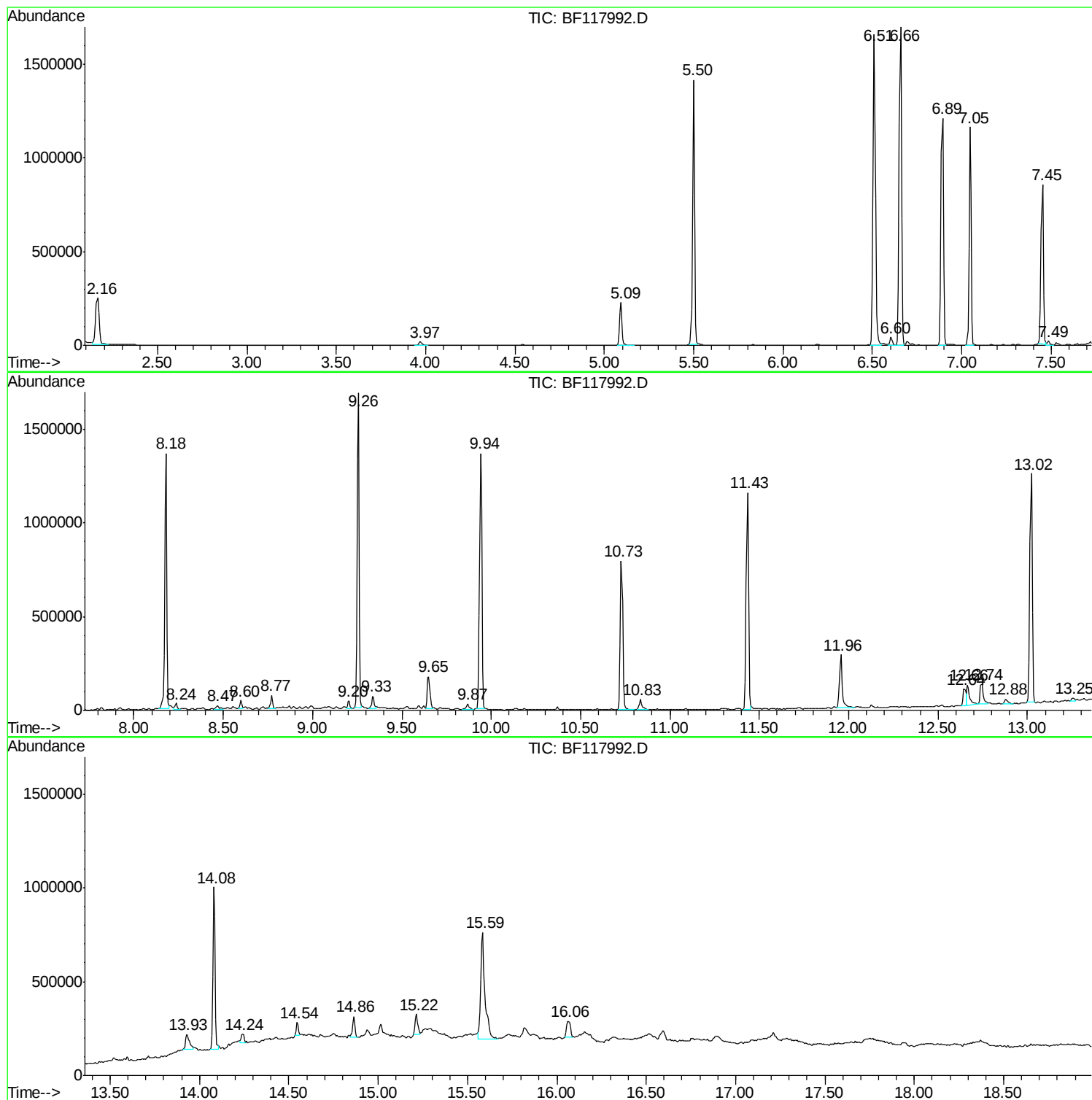
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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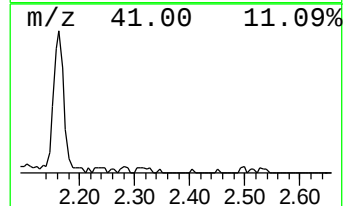
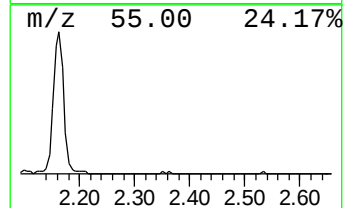
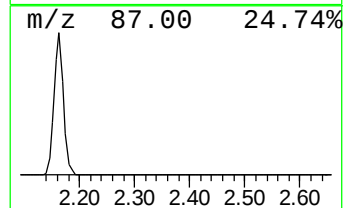
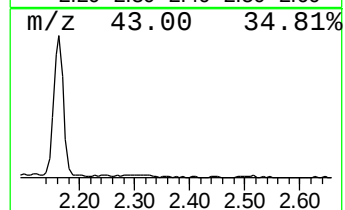
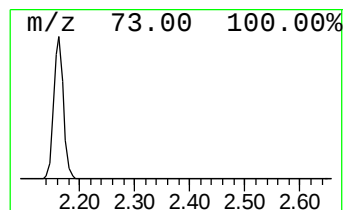
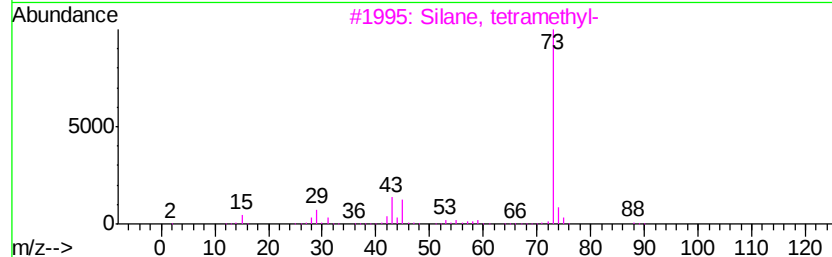
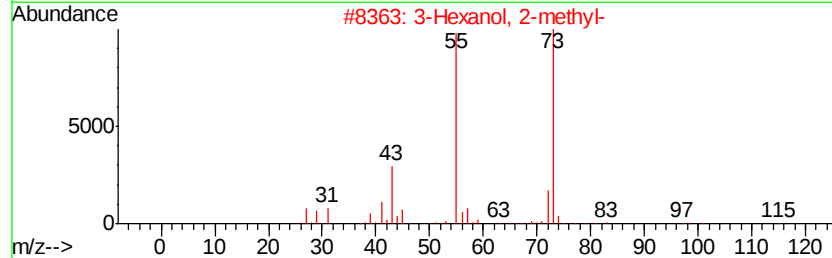
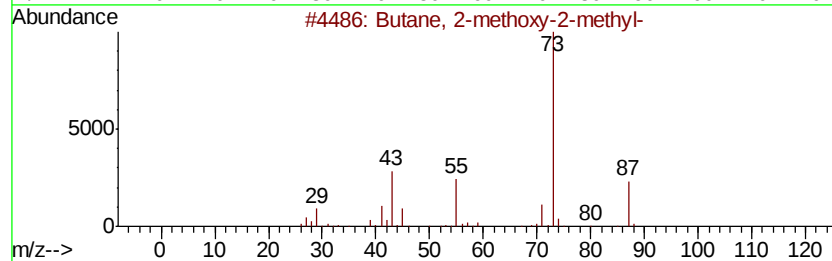
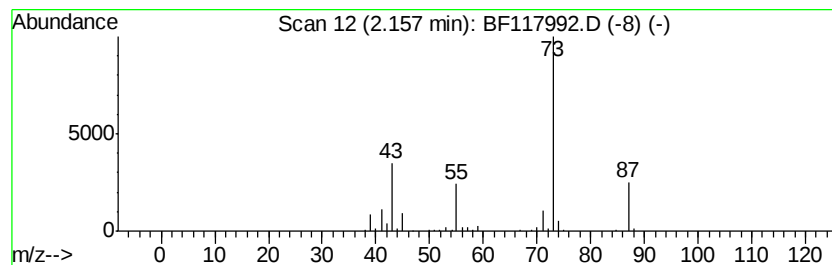
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	5.98 ng	313767	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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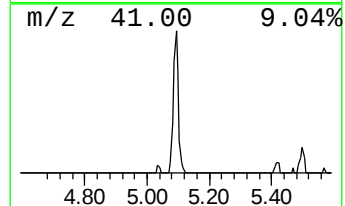
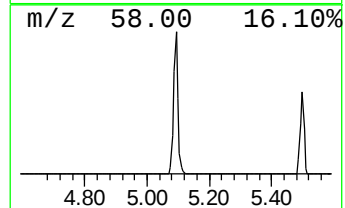
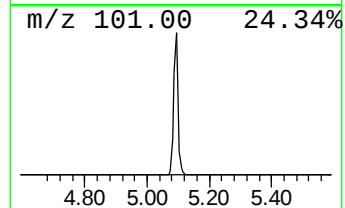
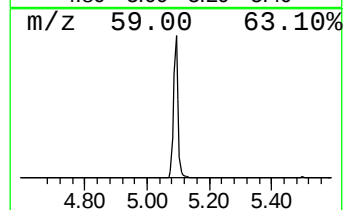
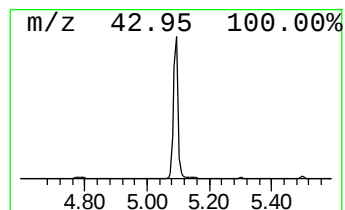
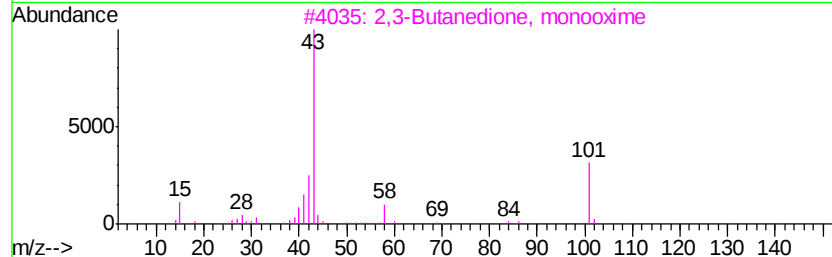
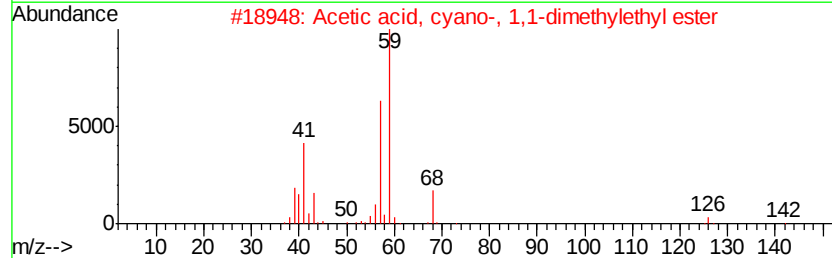
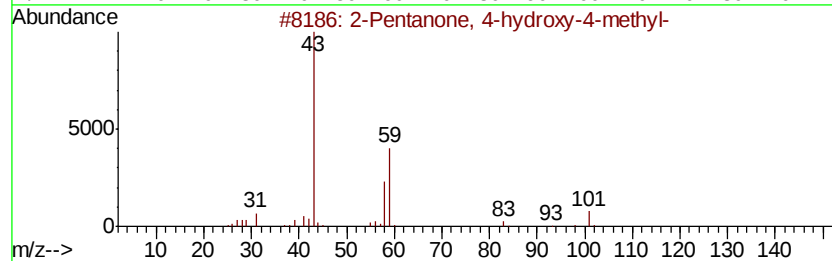
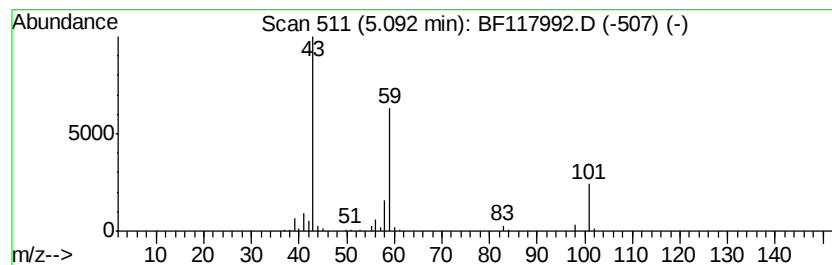
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.41 ng	231310	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Butane	58	C4H10	000106-97-8	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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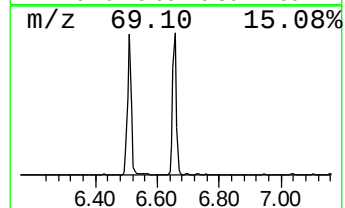
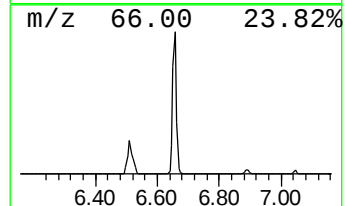
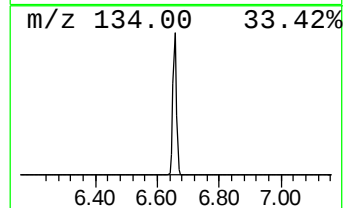
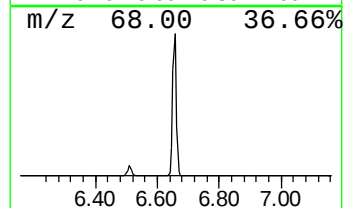
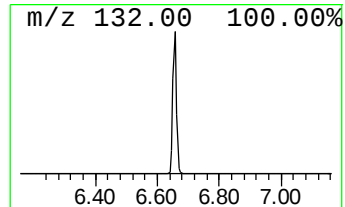
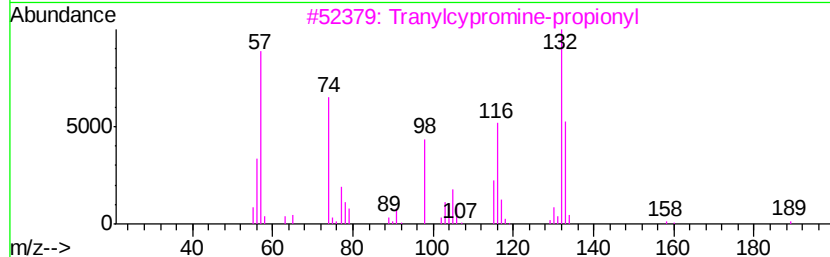
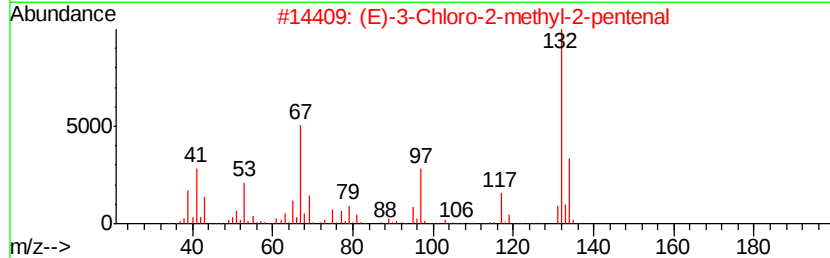
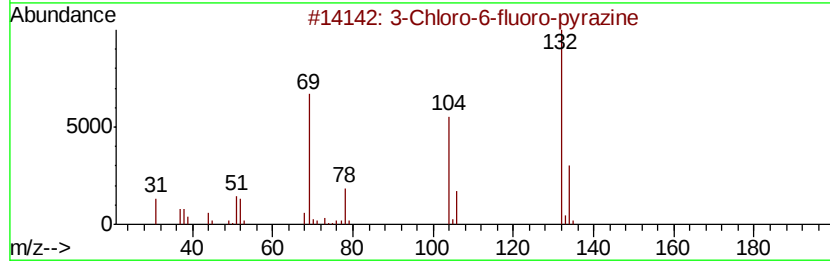
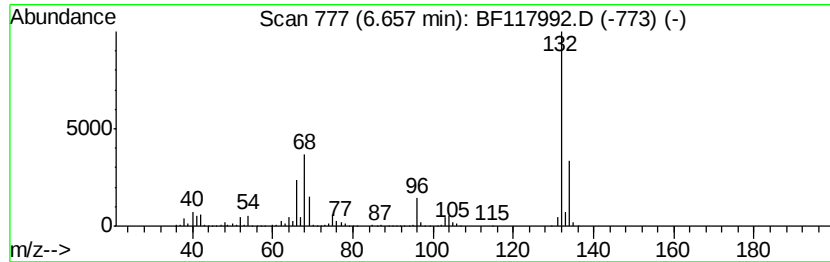
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	26.60 ng	1394540	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	16
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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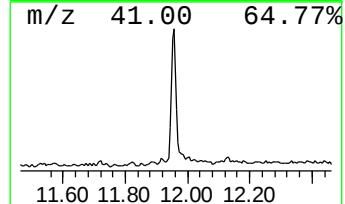
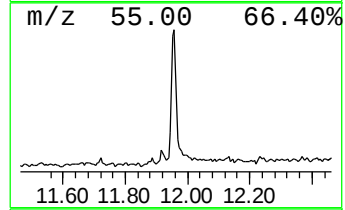
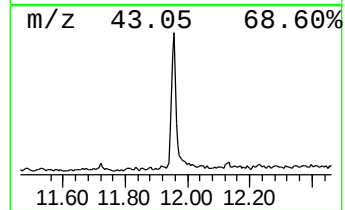
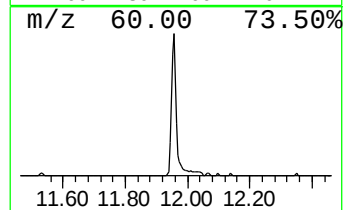
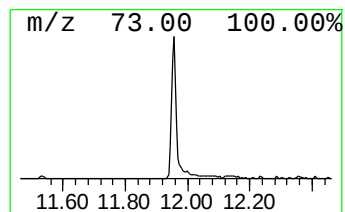
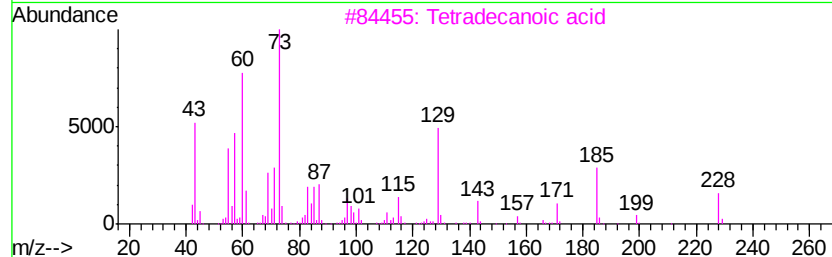
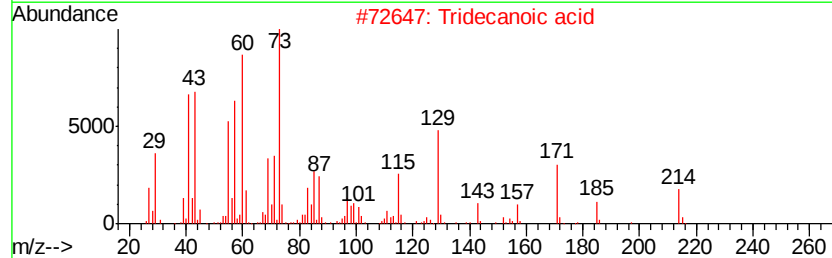
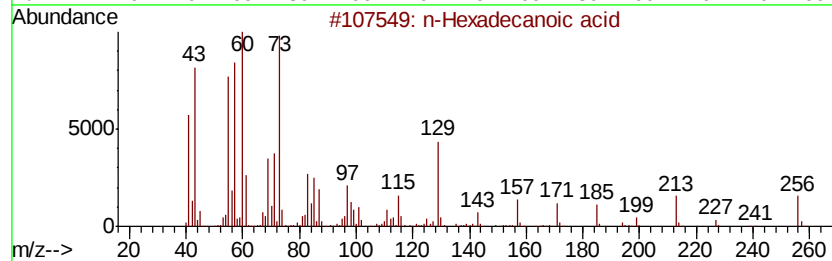
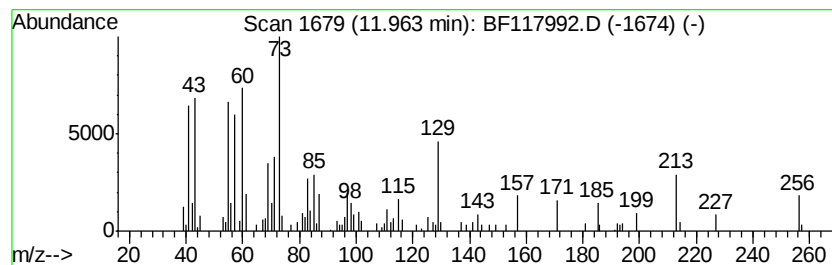
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	6.08 ng	287846	Phenanthrene-d10	11.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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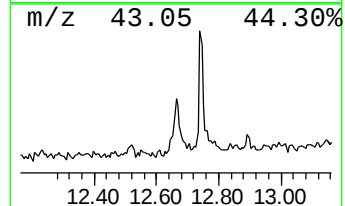
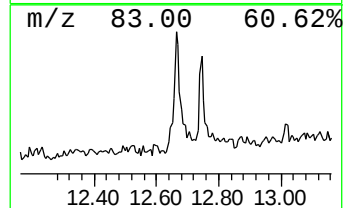
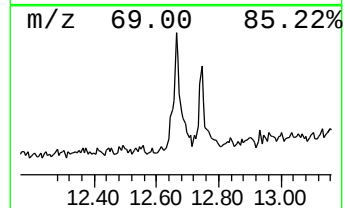
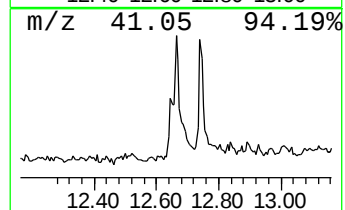
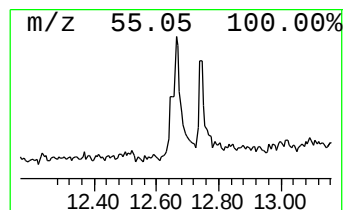
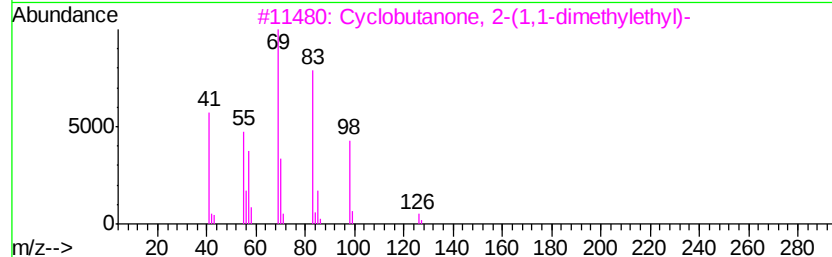
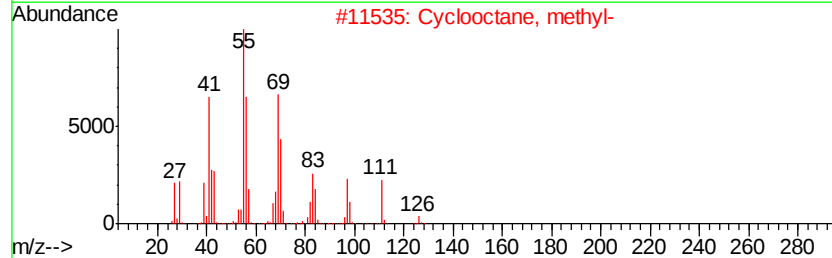
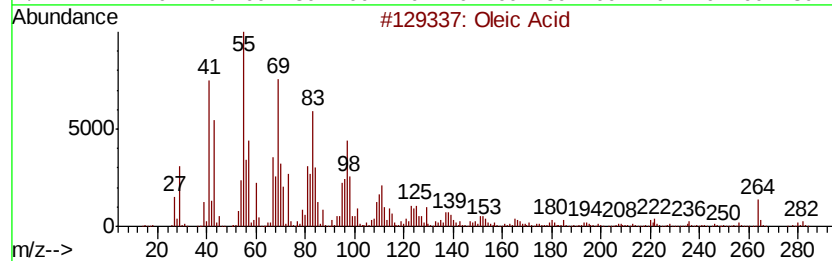
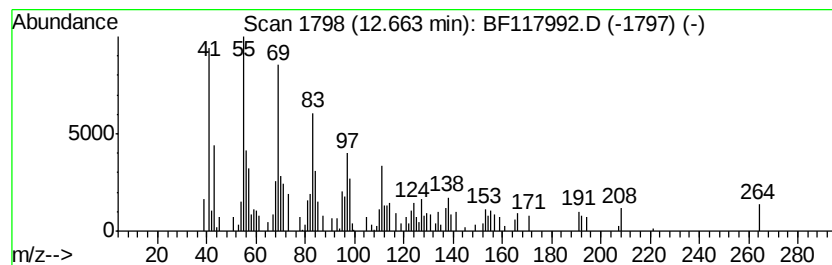
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oleic Acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.66	2.65 ng	125578	Phenanthrene-d10	11.43		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oleic Acid	282	C18H34O2	000112-80-1	90
2		Cyclooctane, methyl-	126	C9H18	001502-38-1	58
3		Cyclobutanone, 2-(1,1-dimethylet...	126	C8H14O	004579-31-1	50
4		Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	50
5		4-Methyl-dodec-3-en-1-ol	198	C13H26O	1000192-41-0	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117992.D
Acq On : 26 Nov 2019 3:36
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PHIPPS-BH-NW-01

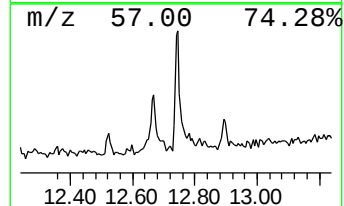
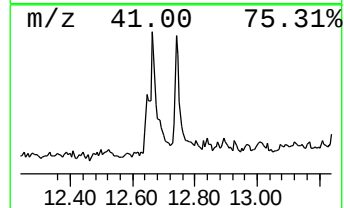
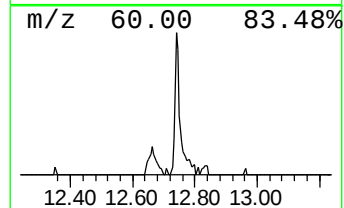
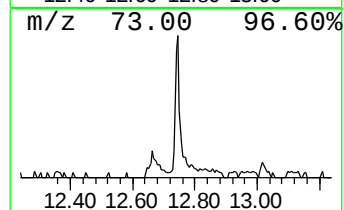
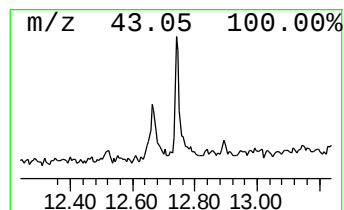
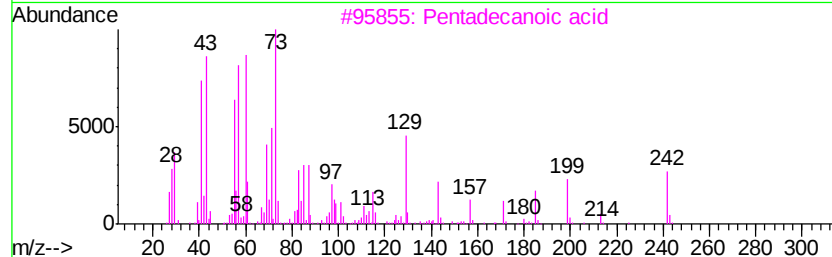
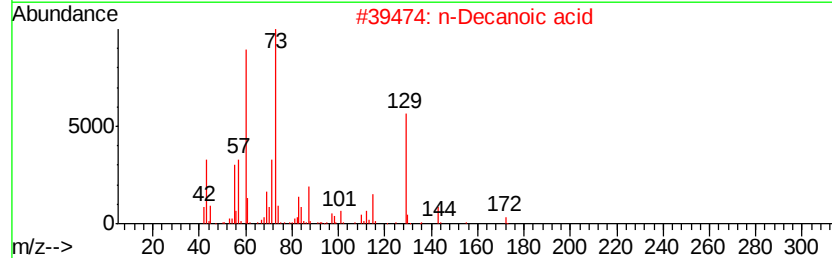
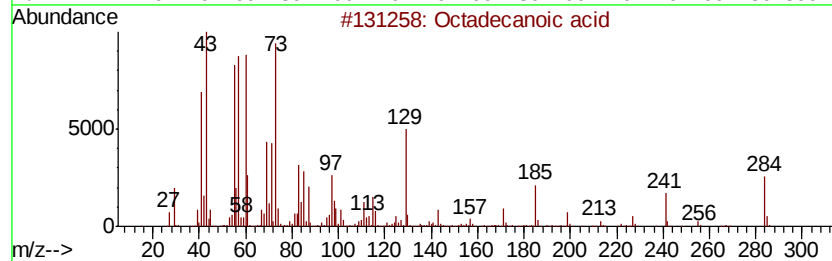
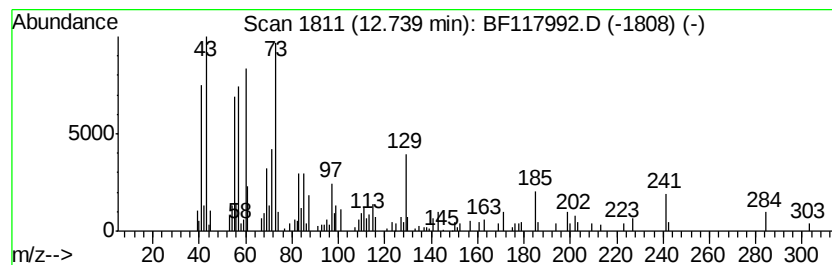
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.64 ng	124825	Phenanthrene-d10	11.43

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Decanoic acid	172	C10H20O2	000334-48-5	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117992.D
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Misc :
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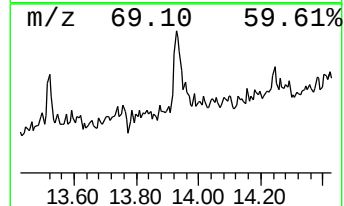
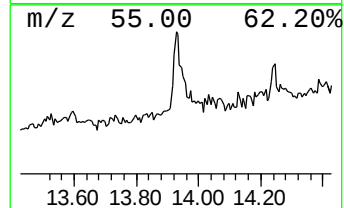
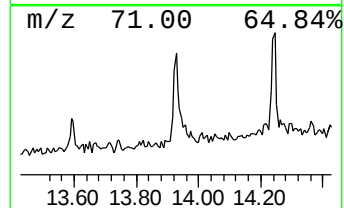
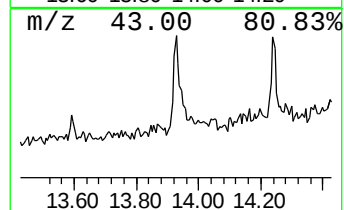
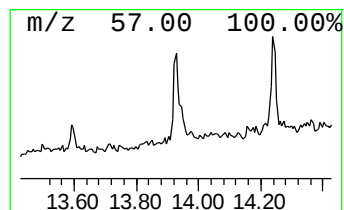
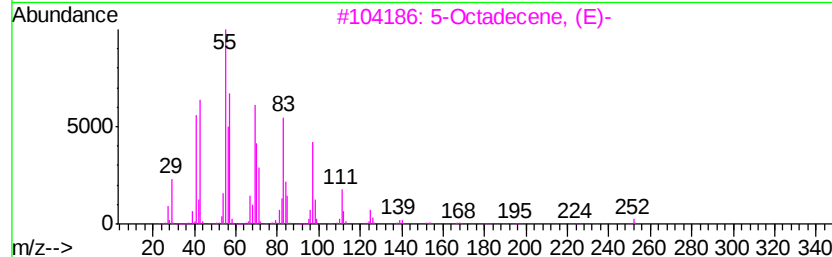
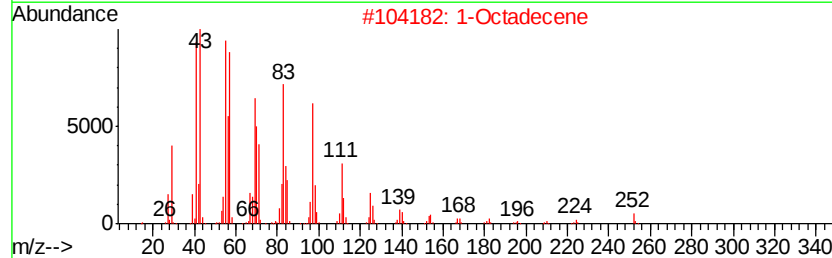
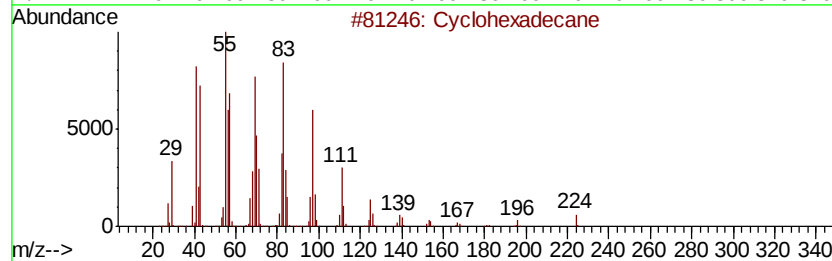
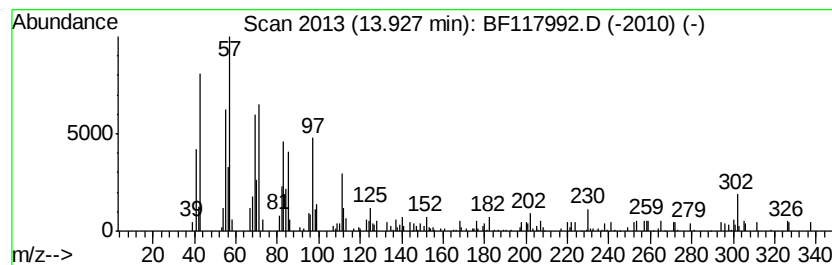
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.45 ng	135431	Chrysene-d12	14.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexadecane	224	C16H32	000295-65-8	96
2		1-Octadecene	252	C18H36	000112-88-9	95
3		5-Octadecene, (E)-	252	C18H36	007206-21-5	89
4		Cetene	224	C16H32	000629-73-2	89
5		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
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Acq On : 26 Nov 2019 3:36
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Sample : K5839-01 2X
Misc :
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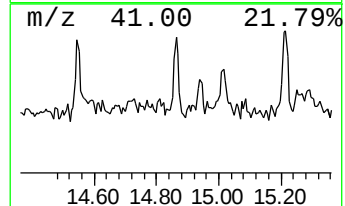
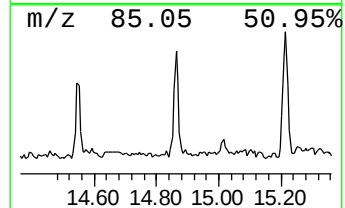
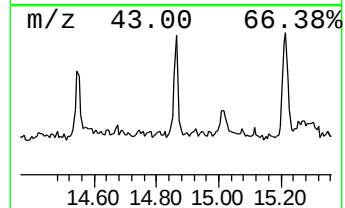
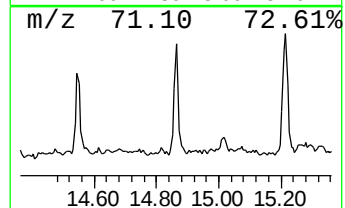
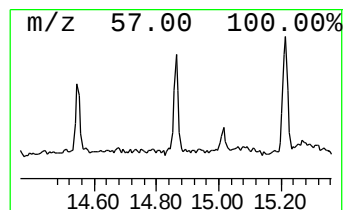
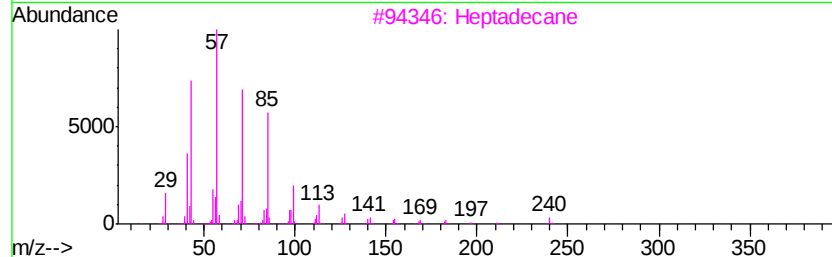
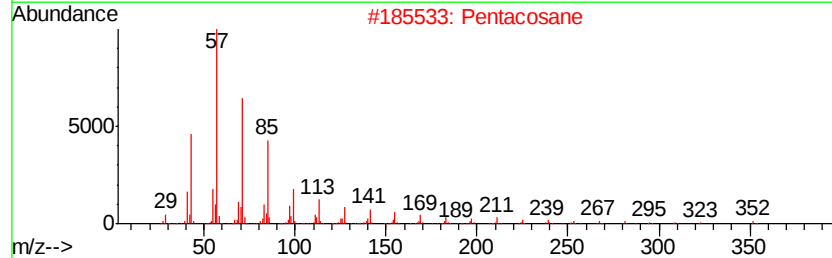
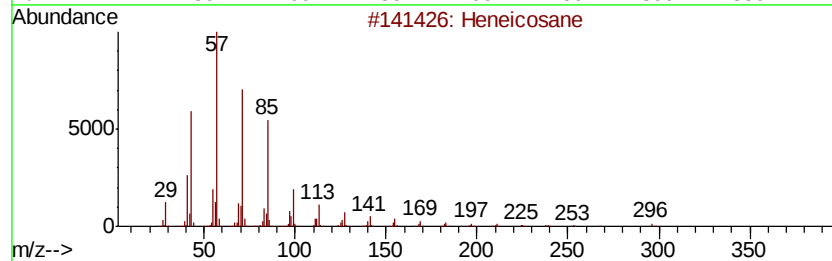
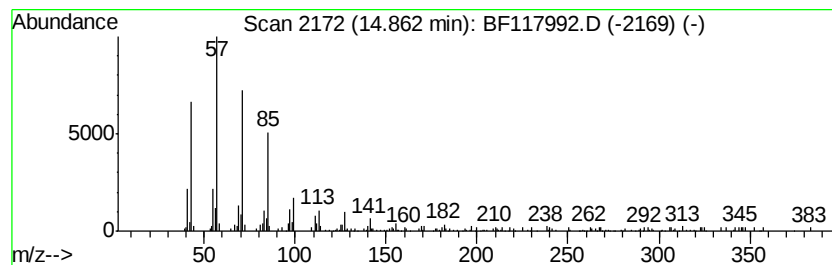
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	2.30 ng	108477	Perylene-d12	15.59
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	99
2	Pentacosane	352 C25H52	000629-99-2	96
3	Heptadecane	240 C17H36	000629-78-7	94
4	Tetracosane	338 C24H50	000646-31-1	91
5	triacontane	422 C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117992.D
Acq On : 26 Nov 2019 3:36
Operator : JU
Sample : K5839-01 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

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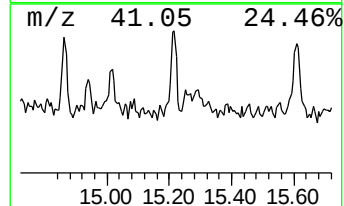
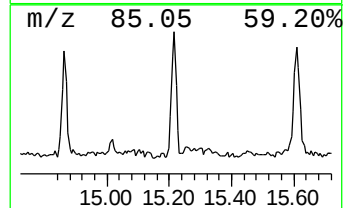
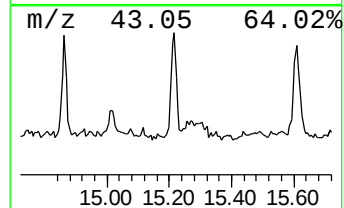
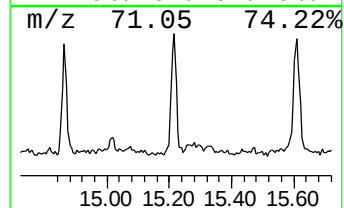
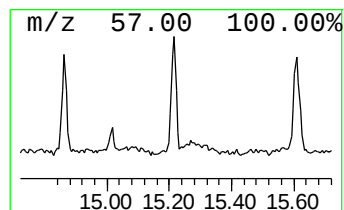
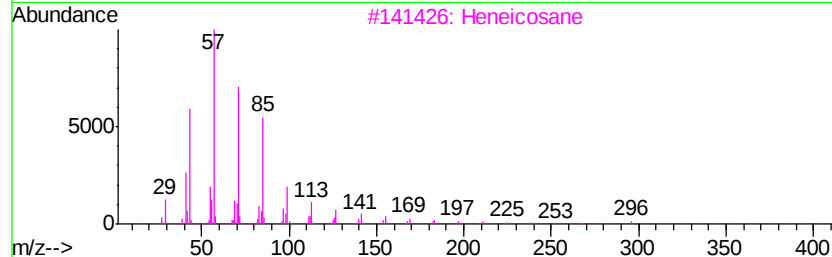
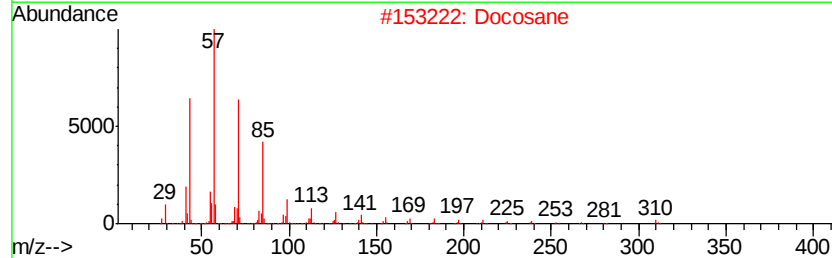
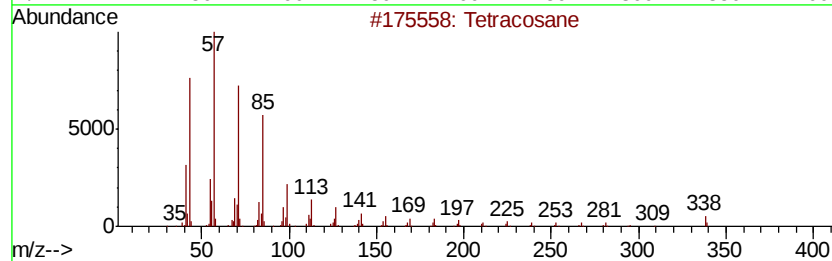
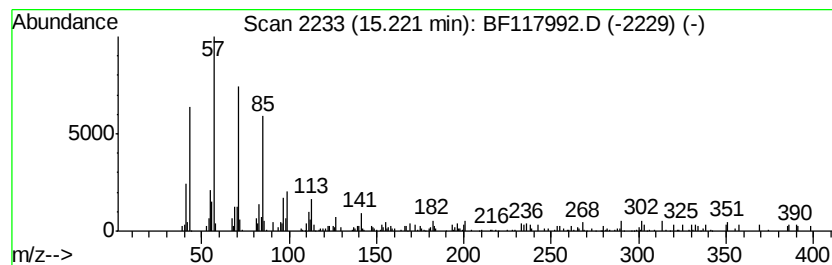
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.39 ng	112620	Perylene-d12	15.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	97
2			Docosane	310	C22H46	000629-97-0	95
3			Heneicosane	296	C21H44	000629-94-7	90
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			2-methyloctacosane	408	C29H60	1000376-72-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117992.D
Acq On : 26 Nov 2019 3:36
Operator : JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

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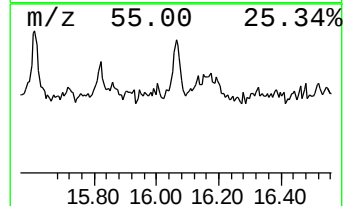
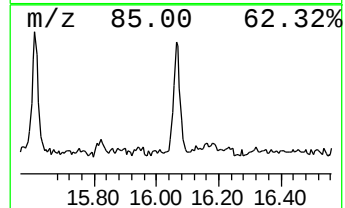
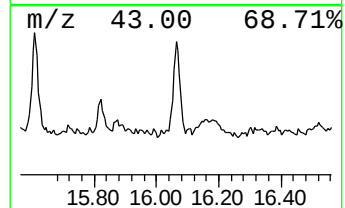
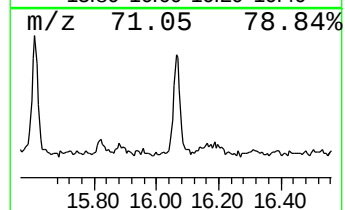
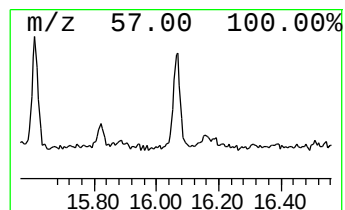
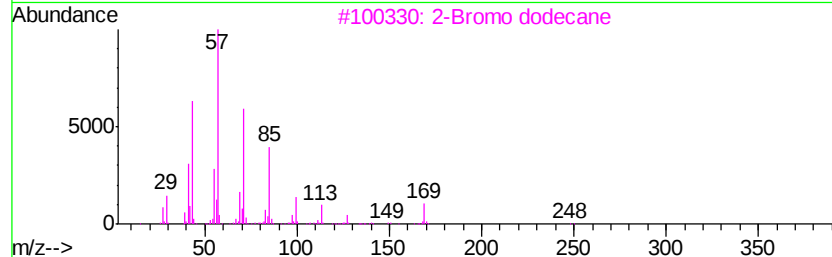
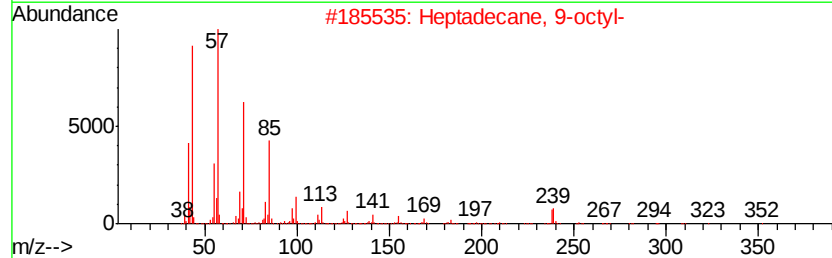
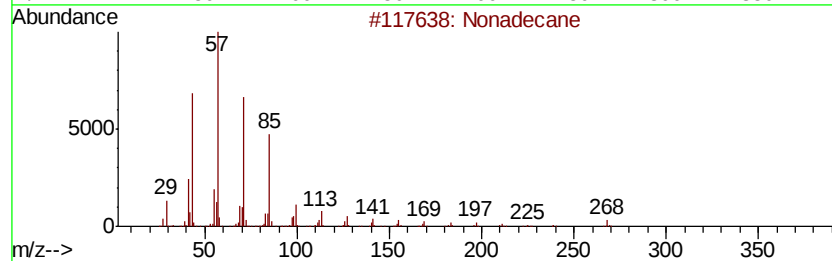
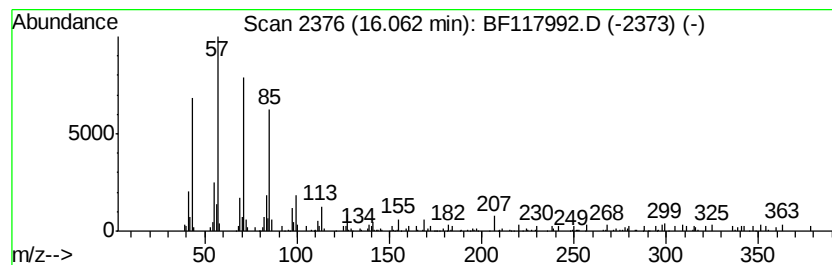
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	2.47 ng	116297	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	90
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	87
4		triacontane	422	C30H62	000638-68-6	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112519\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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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...	5.09	4.4	ng	231310	1	6.89	1048580	20.0
unknown6.66	6.66	26.6	ng	1394540	1	6.89	1048580	20.0
n-Hexadecanoic acid	11.96	6.1	ng	287846	4	11.43	947429	20.0
Oleic Acid	12.66	2.6	ng	125578	4	11.43	947429	20.0
Octadecanoic acid	12.74	2.6	ng	124825	4	11.43	947429	20.0
Cyclohexadecane	13.93	3.5	ng	135431	5	14.08	785487	20.0
Heneicosane	14.86	2.3	ng	108477	6	15.59	942303	20.0
Tetracosane	15.22	2.4	ng	112620	6	15.59	942303	20.0
Nonadecane	16.06	2.5	ng	116297	6	15.59	942303	20.0