

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112519\
 Data File : BF117995.D
 Acq On : 26 Nov 2019 5:01
 Operator : JU
 Sample : K5840-09 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PHIPPS-BH-SE-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	2.140	4	9	25	rVB	334447	438253	38.80%	3.289%
2	5.093	507	511	519	rVB	176129	190181	16.84%	1.427%
3	5.498	576	580	584	rBV	1144320	977639	86.56%	7.337%
4	6.516	749	753	761	rBV	1131211	1072456	94.96%	8.049%
5	6.657	773	777	781	rBV	1317389	1078578	95.50%	8.095%
6	6.892	813	817	820	rBV	892684	694623	61.50%	5.213%
7	7.045	840	843	847	rBV	968344	871567	77.17%	6.541%
8	7.451	908	912	915	rBV	731473	586541	51.93%	4.402%
9	8.181	1029	1036	1039	rBV	1057678	861622	76.29%	6.466%
10	8.239	1043	1046	1049	rVB	17898	15211	1.35%	0.114%
11	8.598	1105	1107	1109	rBV	19816	15342	1.36%	0.115%
12	8.769	1133	1136	1141	rBV	44251	35860	3.18%	0.269%
13	9.092	1181	1191	1195	rBV7	8471	20609	1.82%	0.155%
14	9.204	1207	1210	1215	rVB2	24072	22385	1.98%	0.168%
15	9.257	1215	1219	1222	rBV	1543807	1129413	100.00%	8.476%
16	9.339	1230	1233	1235	rBV	45829	39941	3.54%	0.300%
17	9.651	1283	1286	1290	rVB	111106	98334	8.71%	0.738%
18	9.869	1318	1323	1327	rVB	28954	27571	2.44%	0.207%
19	9.939	1332	1335	1339	rVV	914544	785159	69.52%	5.892%
20	10.133	1365	1368	1375	rBV6	10553	15947	1.41%	0.120%
21	10.369	1406	1408	1411	rVB	22482	17047	1.51%	0.128%
22	10.592	1440	1446	1449	rBV4	11416	15962	1.41%	0.120%
23	10.733	1466	1470	1481	rVB	546377	514412	45.55%	3.861%
24	10.845	1486	1489	1495	rVB2	23027	28829	2.55%	0.216%
25	11.292	1562	1565	1569	rBV	13249	15879	1.41%	0.119%
26	11.433	1585	1589	1593	rBV	834333	695722	61.60%	5.221%
27	11.957	1674	1678	1682	rBV2	93403	98428	8.71%	0.739%
28	12.133	1705	1708	1711	rVB2	21095	18676	1.65%	0.140%
29	12.521	1772	1774	1777	rBV	23209	20780	1.84%	0.156%
30	12.651	1794	1796	1801	rBV2	20015	33433	2.96%	0.251%
31	12.745	1810	1812	1817	rBV4	39054	43870	3.88%	0.329%
32	12.880	1832	1835	1836	rBV2	18196	16820	1.49%	0.126%
33	12.898	1836	1838	1842	rVB2	39480	32473	2.88%	0.244%
34	13.021	1855	1859	1863	rBV	1097026	941645	83.37%	7.067%

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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	13.257	1895	1899	1901	rBV	55804	59010	5.22%	0.443%
36	13.598	1954	1957	1960	rVB	68510	60423	5.35%	0.453%
37	13.927	2010	2013	2020	rBV	126033	179374	15.88%	1.346%
38	14.086	2036	2040	2043	rBV	820748	692770	61.34%	5.199%
39	14.245	2064	2067	2070	rBV	63873	60848	5.39%	0.457%
40	14.551	2116	2119	2123	rBV	86344	82548	7.31%	0.620%
41	14.863	2170	2172	2177	rVB	64400	61093	5.41%	0.458%
42	14.945	2183	2186	2189	rVB	66491	68042	6.02%	0.511%
43	15.215	2229	2232	2235	rBV	65439	75149	6.65%	0.564%
44	15.586	2291	2295	2299	rBV	412114	514300	45.54%	3.860%

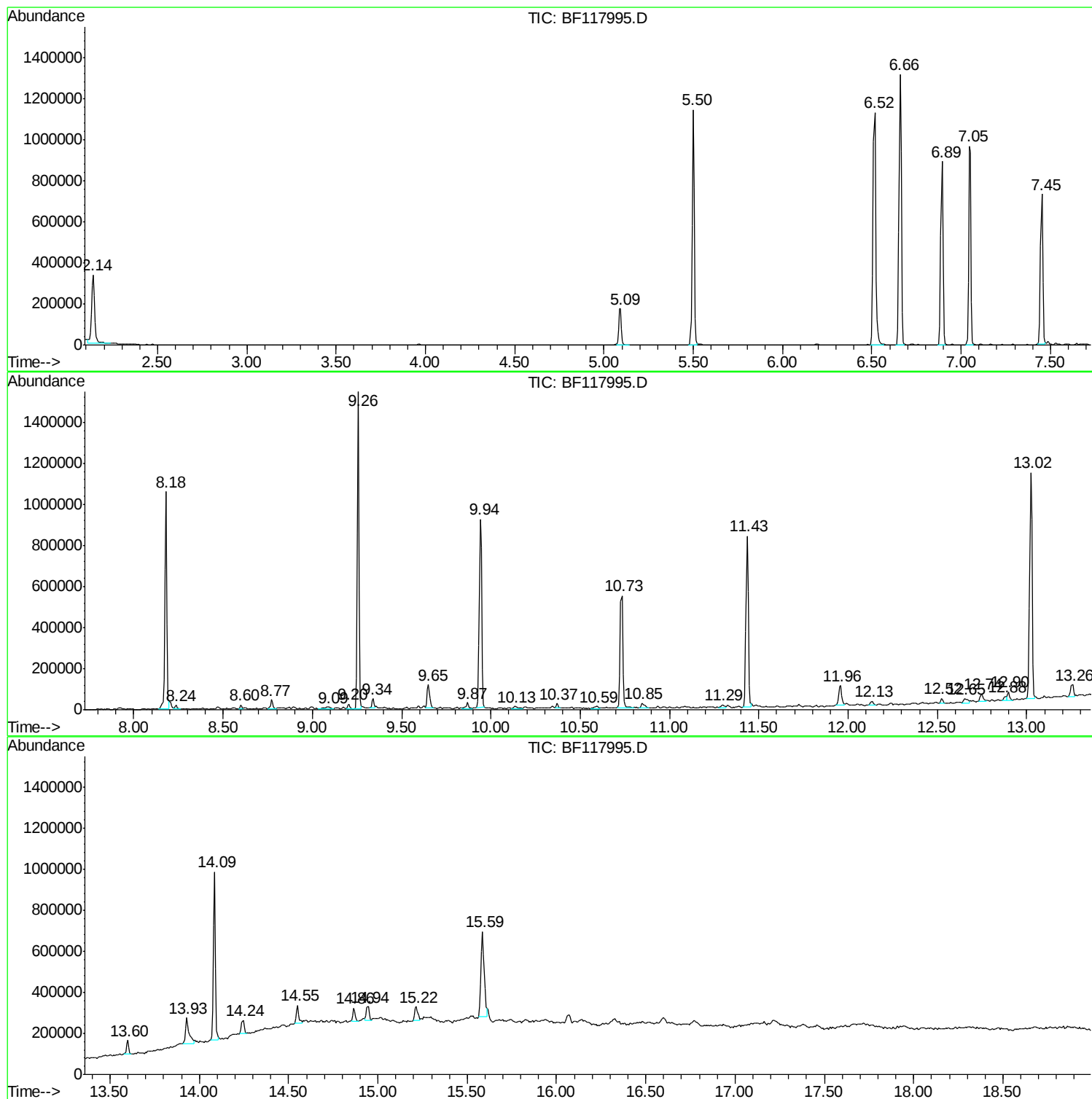
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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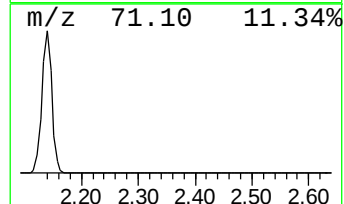
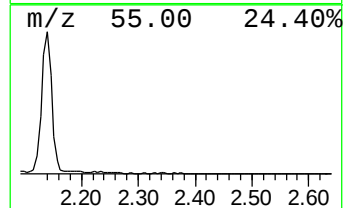
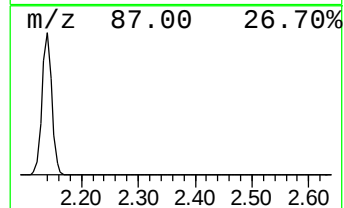
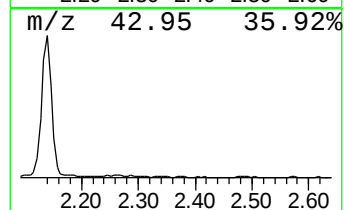
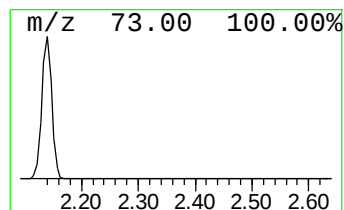
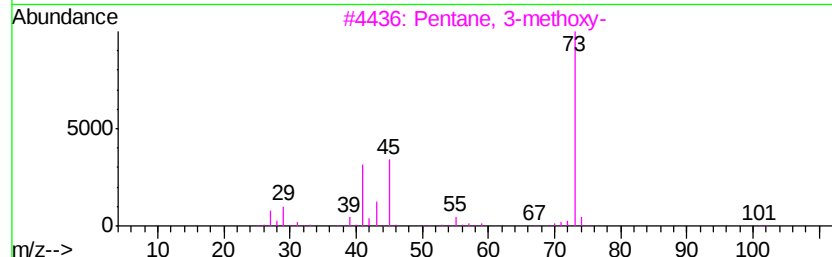
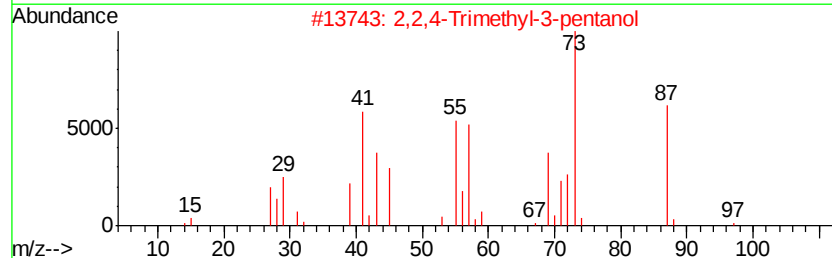
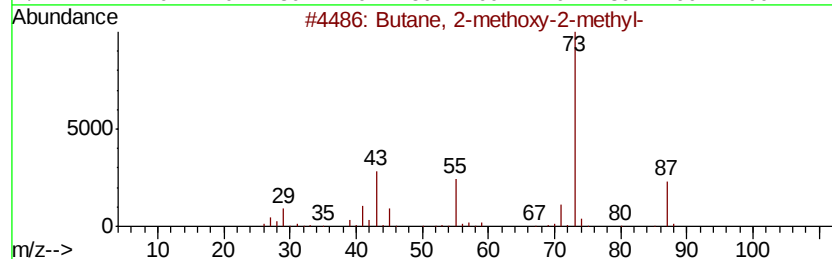
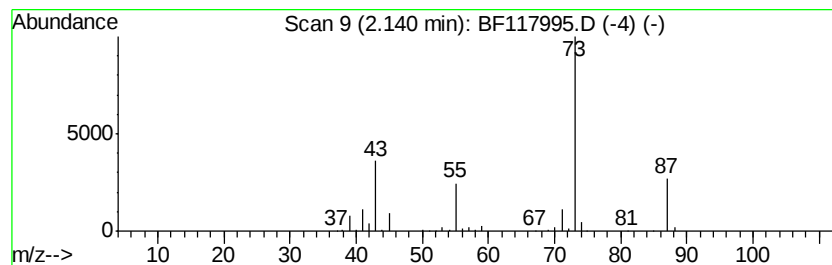
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	12.62 ng	438253	1,4-Dichlorobenzene-d4	6.89

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	56
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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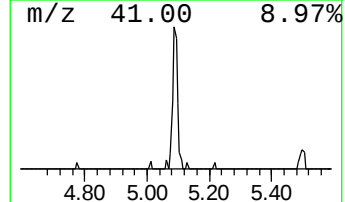
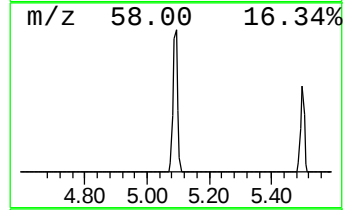
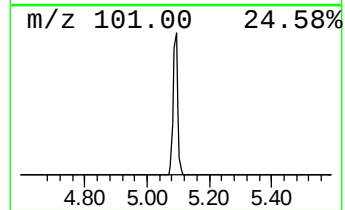
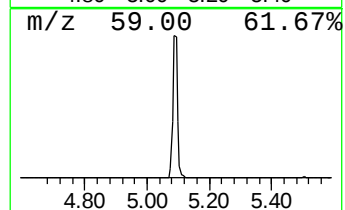
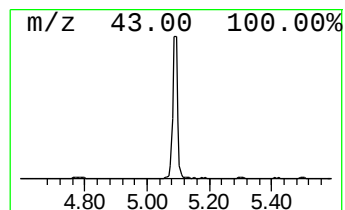
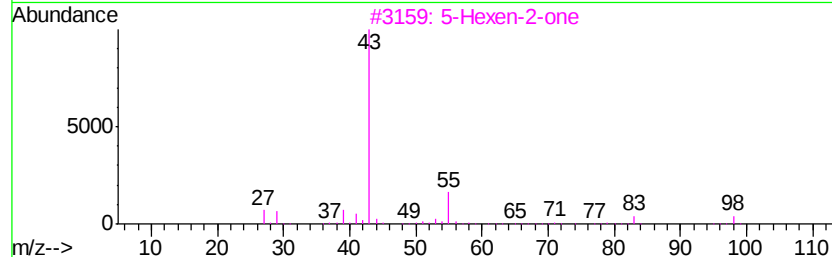
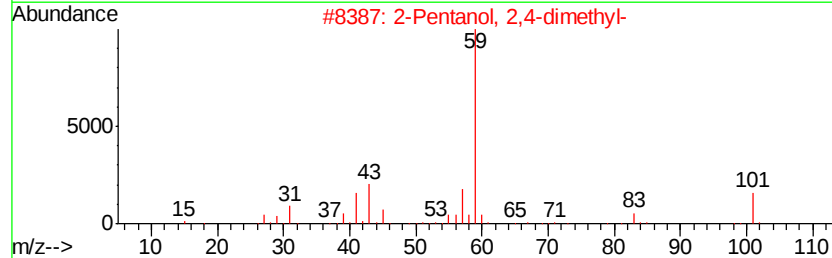
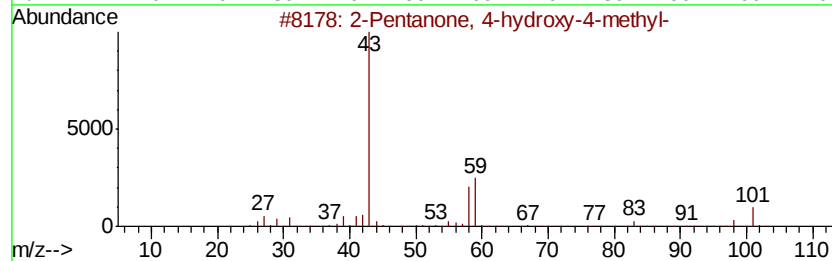
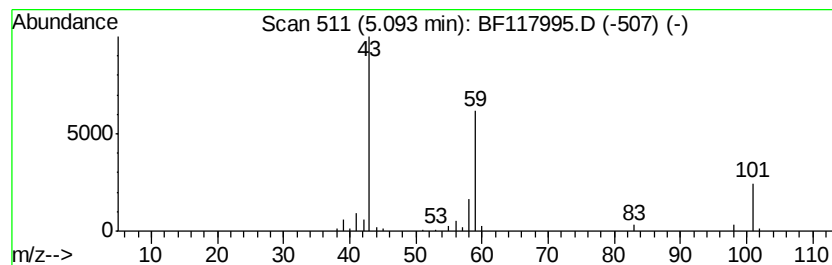
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	5.48 ng	190181	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	36
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Acetone	58	C3H6O	000067-64-1	9



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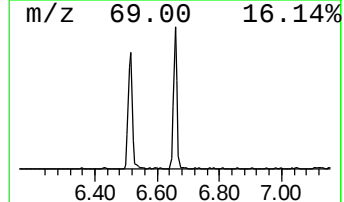
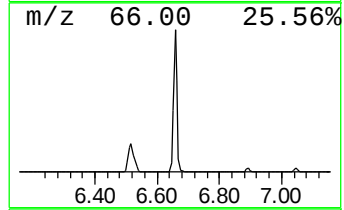
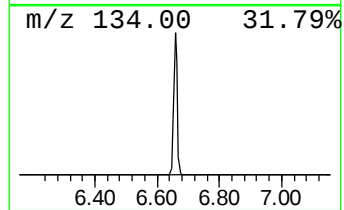
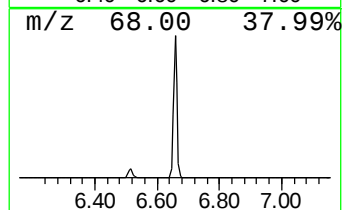
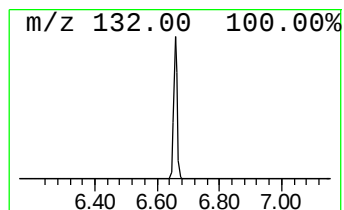
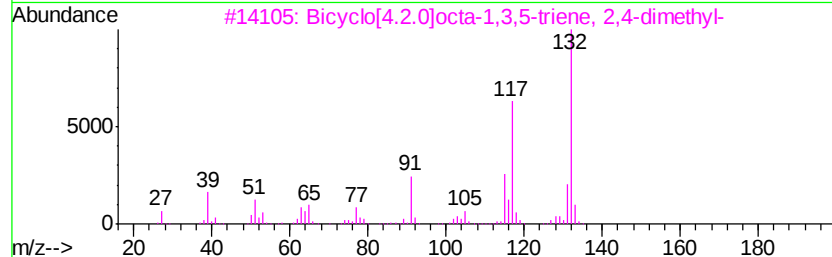
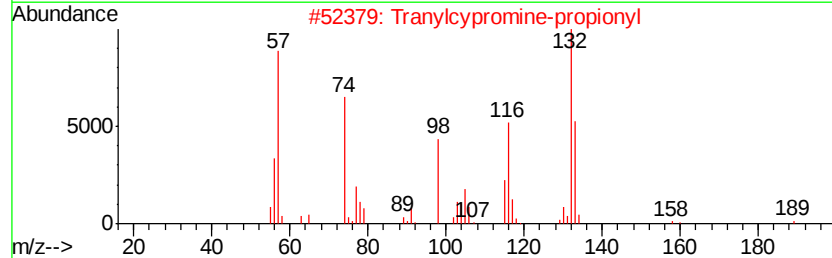
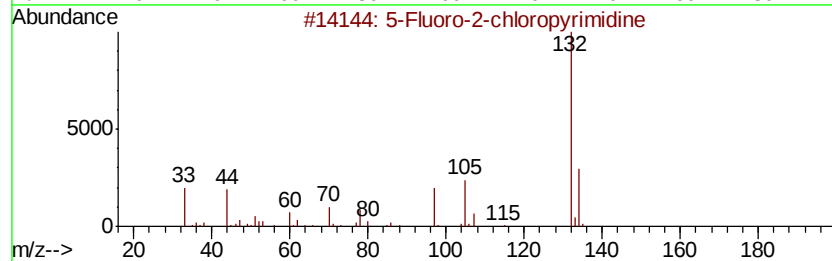
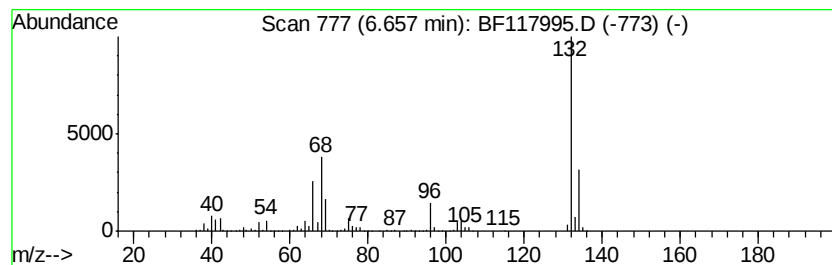
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	31.06 ng	1078580	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
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		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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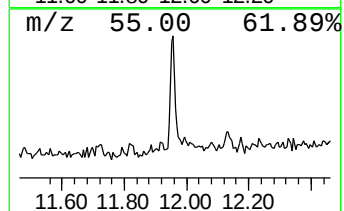
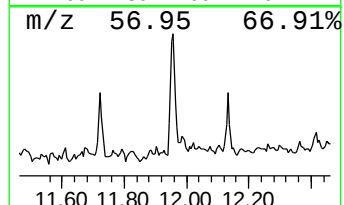
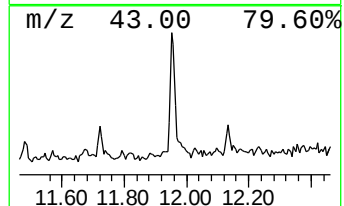
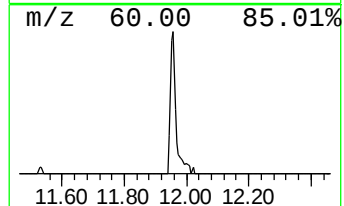
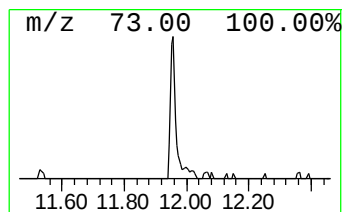
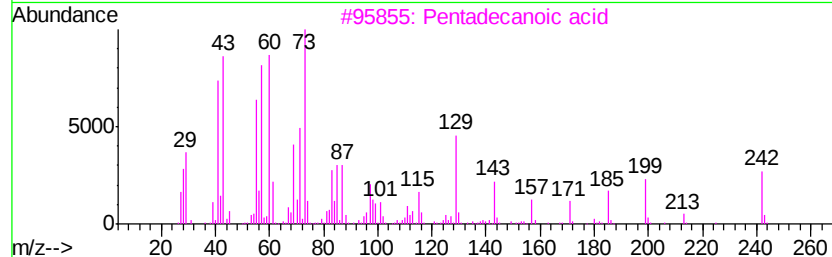
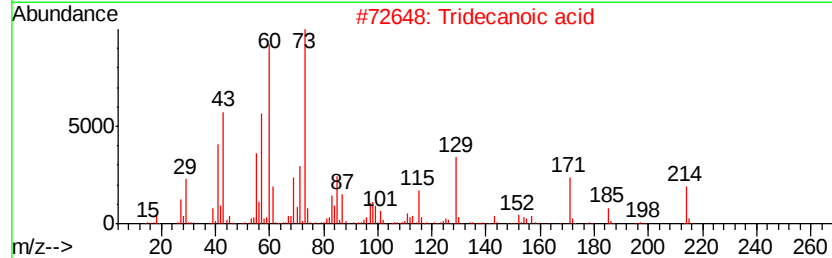
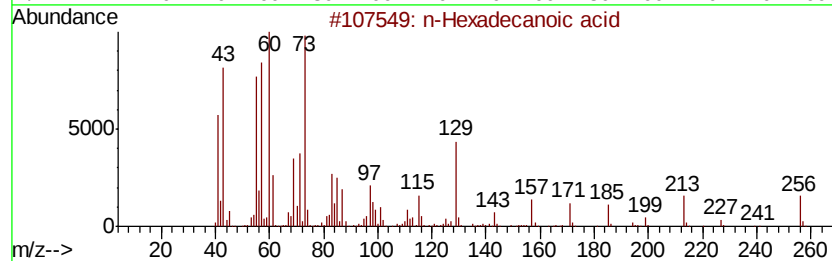
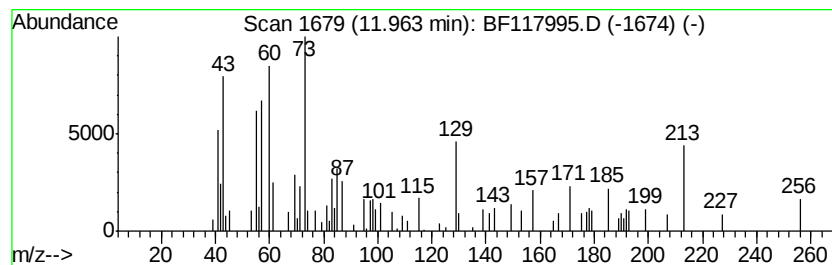
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	2.83 ng	98428	Phenanthrene-d10	11.43

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		Undecanoic acid	186	C11H22O2	000112-37-8	64
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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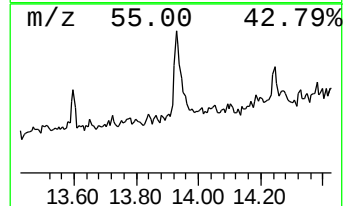
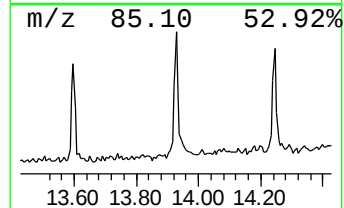
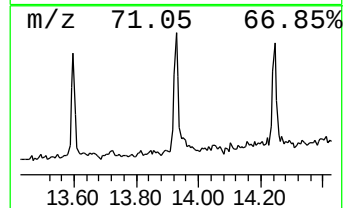
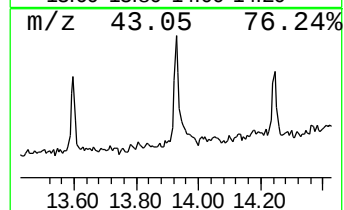
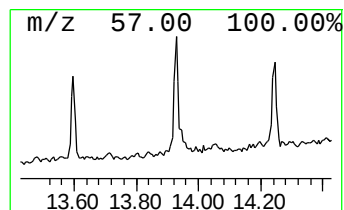
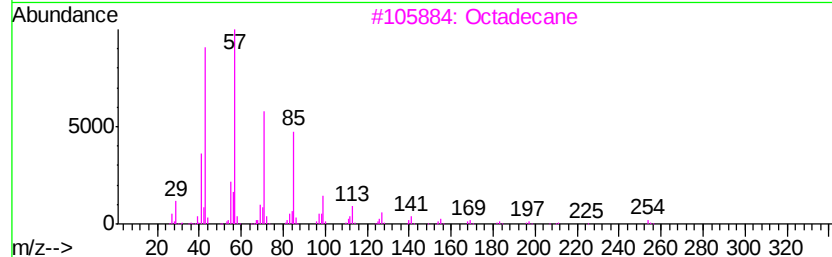
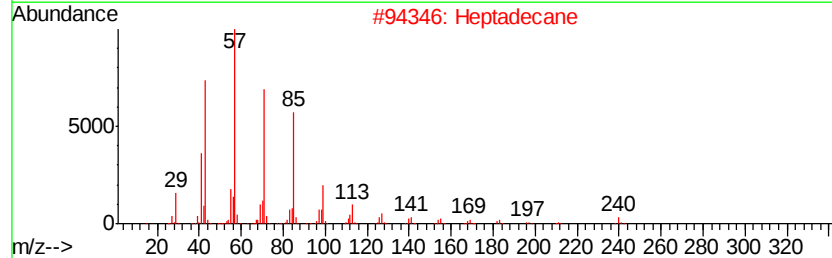
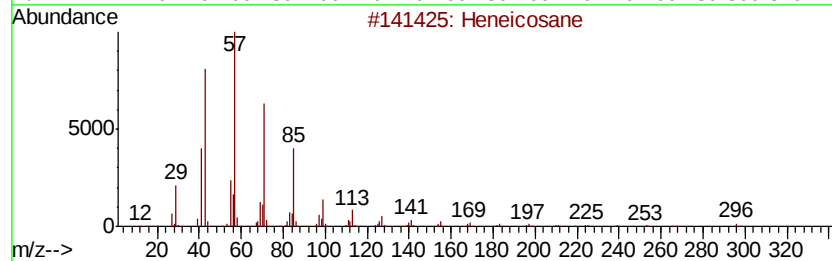
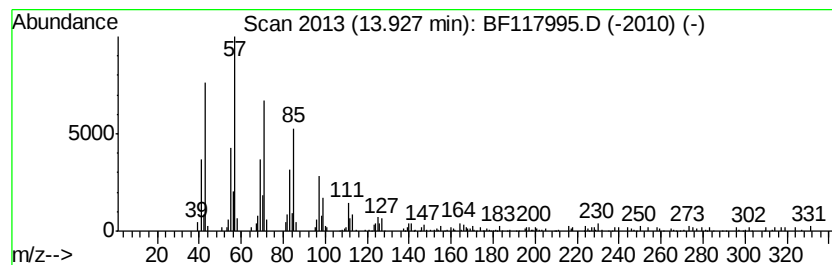
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	5.18 ng	179374	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Heptadecane	240	C17H36	000629-78-7	95
3	Octadecane	254	C18H38	000593-45-3	93
4	Nonadecane, 1-chloro-	302	C19H39Cl	062016-76-6	93
5	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117995.D
Acq On : 26 Nov 2019 5:01
Operator : JU
Sample : K5840-09 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

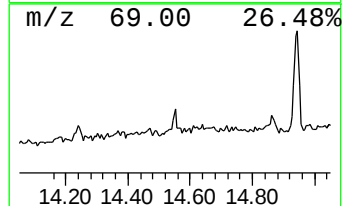
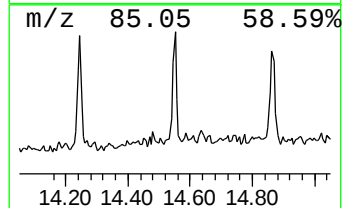
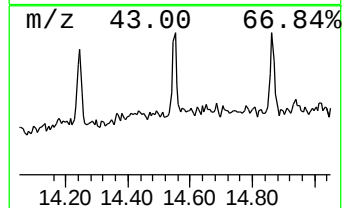
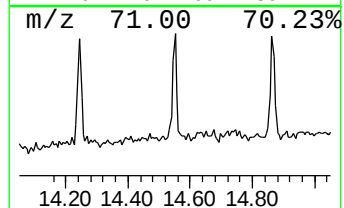
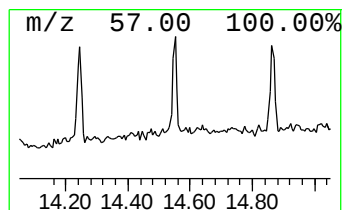
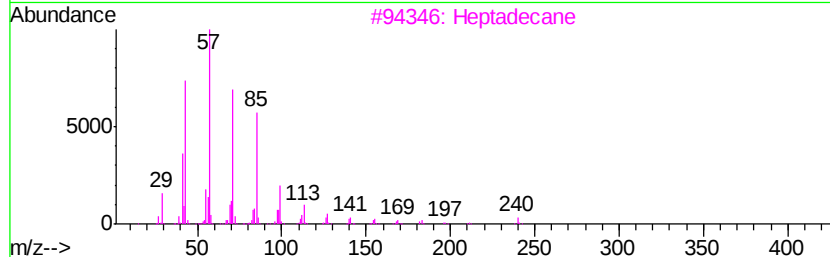
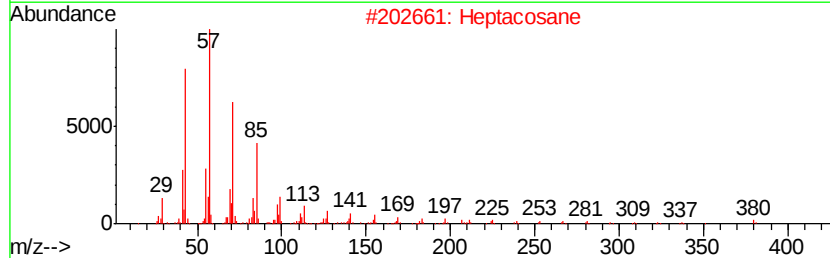
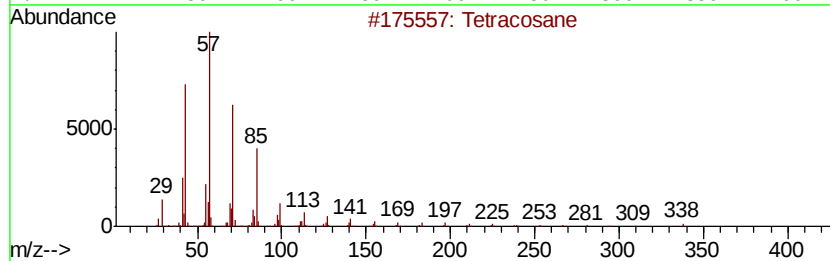
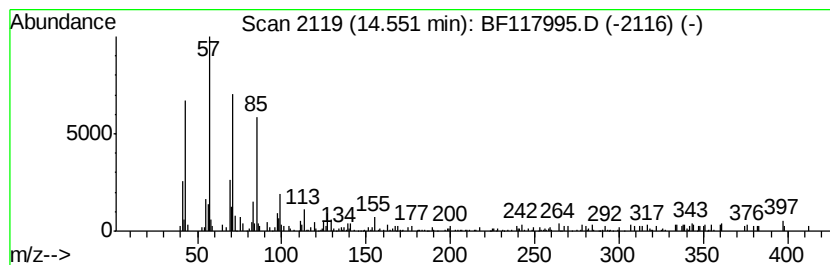
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	2.38 ng	82548	Chrysene-d12	14.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	89
2		Heptacosane	380	C27H56	000593-49-7	86
3		Heptadecane	240	C17H36	000629-78-7	86
4		Eicosane	282	C20H42	000112-95-8	86
5		Octadecane	254	C18H38	000593-45-3	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117995.D
Acq On : 26 Nov 2019 5:01
Operator : JU
Sample : K5840-09 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

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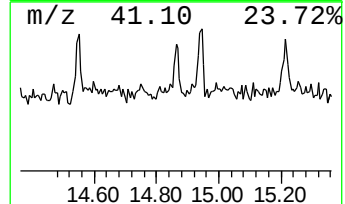
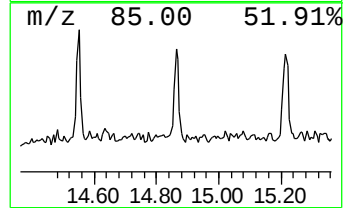
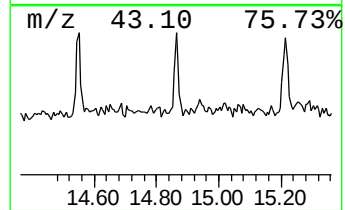
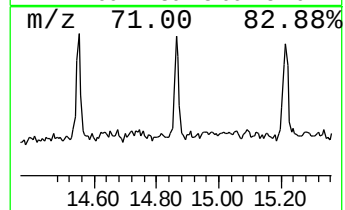
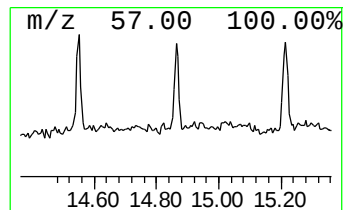
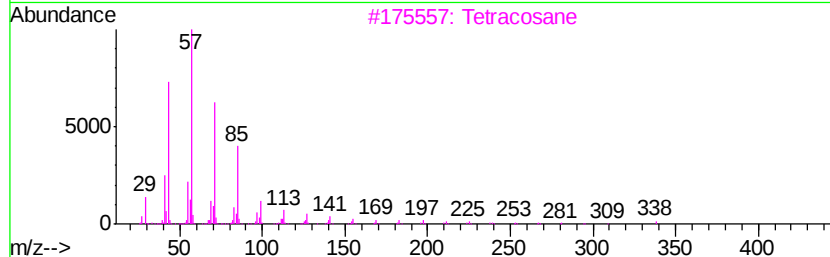
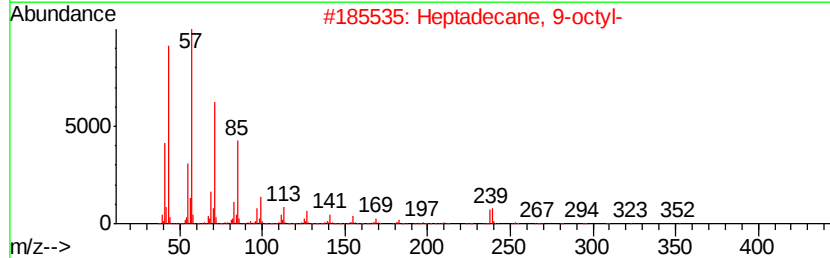
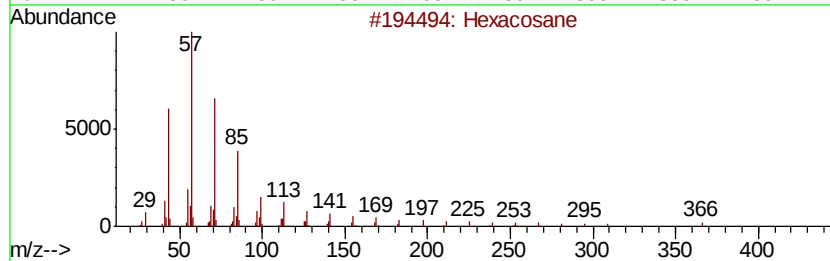
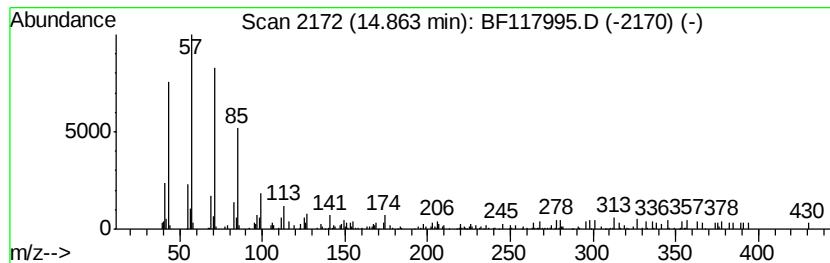
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	2.38 ng	61093	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	93
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3		Tetracosane	338	C24H50	000646-31-1	89
4		Eicosane	282	C20H42	000112-95-8	89
5		Heneicosane	296	C21H44	000629-94-7	89



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117995.D
Acq On : 26 Nov 2019 5:01
Operator : JU
Sample : K5840-09 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

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

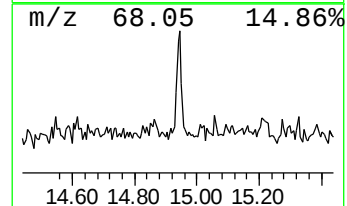
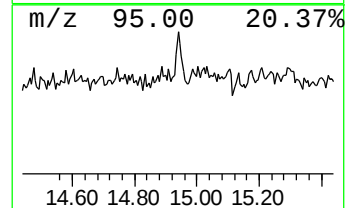
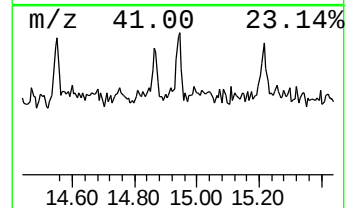
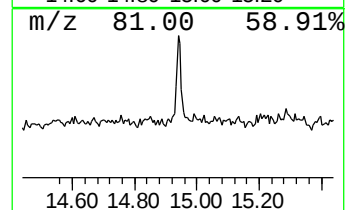
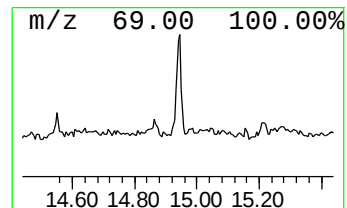
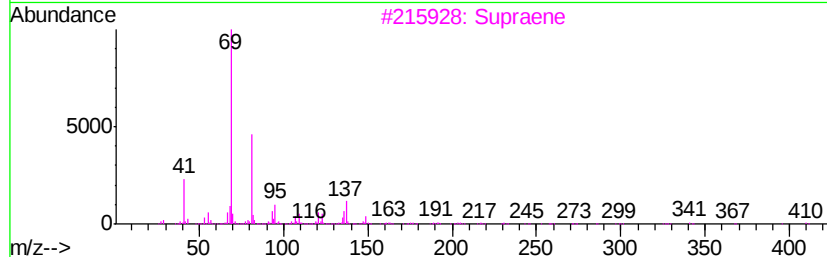
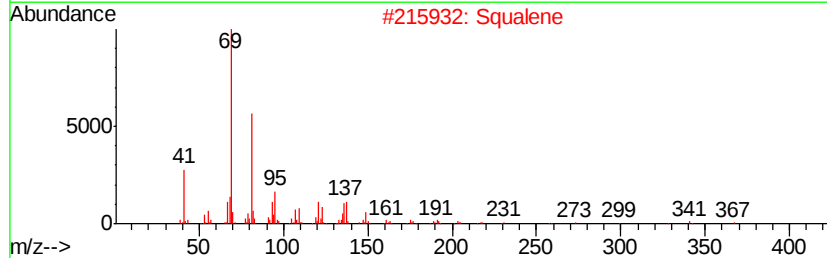
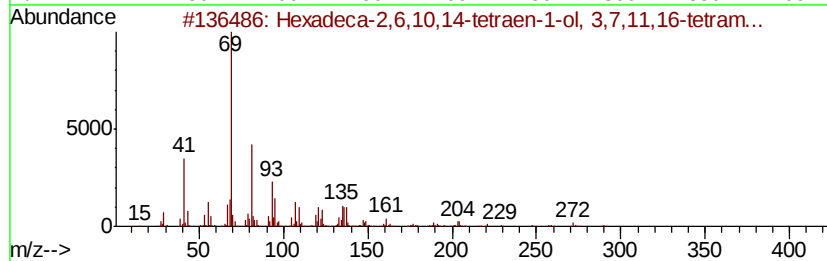
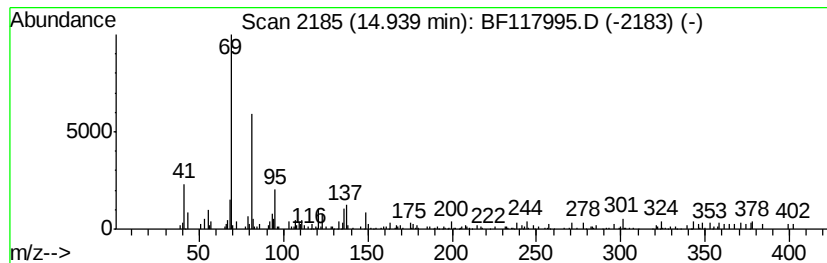
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadeca-2,6,10,14-tetraen-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	2.65 ng	68042	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	87
2		Squalene	410	C30H50	000111-02-4	83
3		Supraene	410	C30H50	007683-64-9	74
4		Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112519\
Data File : BF117995.D
Acq On : 26 Nov 2019 5:01
Operator : JU
Sample : K5840-09 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

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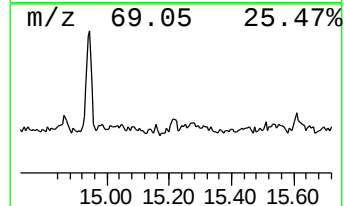
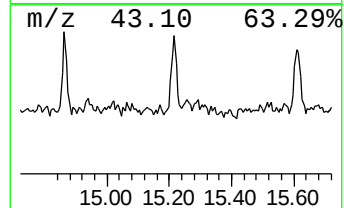
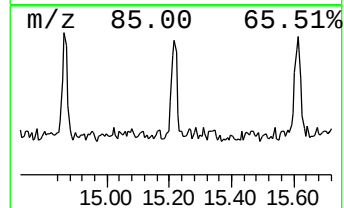
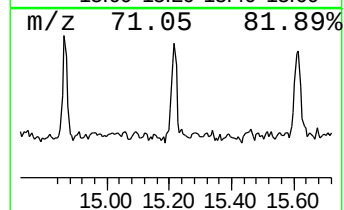
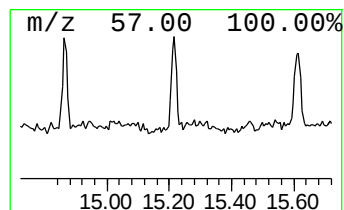
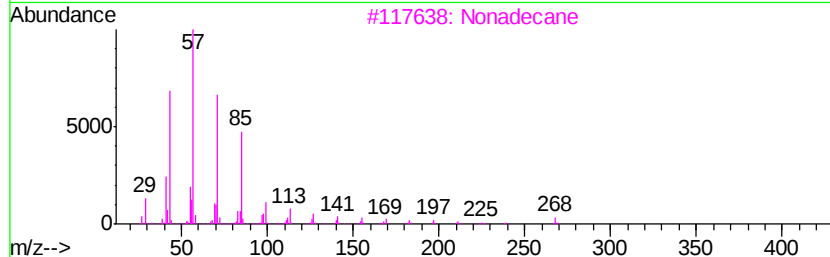
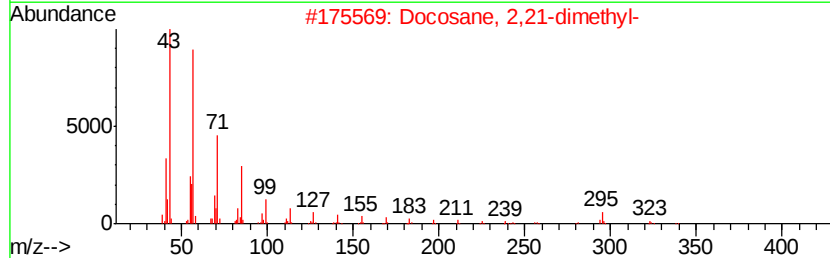
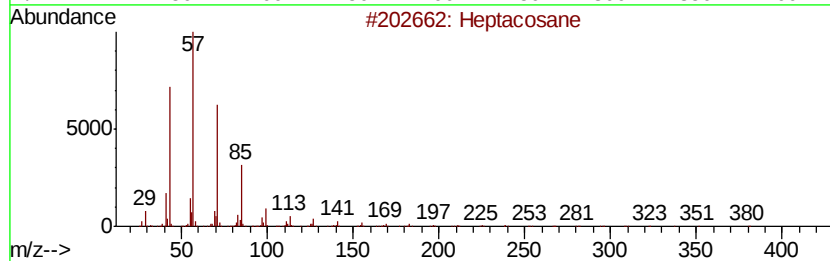
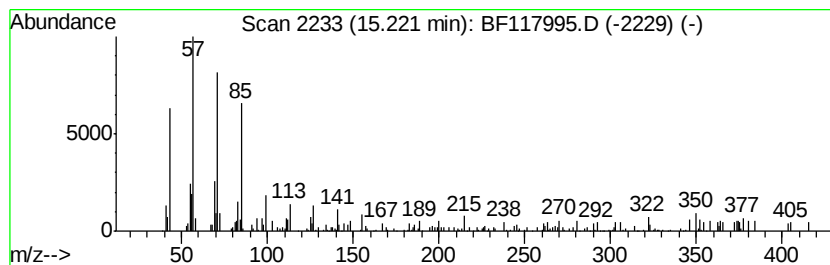
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane, 2,21-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.92 ng	75149	Perylene-d12	15.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	93
2		Docosane, 2,21-dimethyl-	338	C24H50	077536-31-3	92
3		Nonadecane	268	C19H40	000629-92-5	92
4		Heneicosane	296	C21H44	000629-94-7	86
5		Tricosane	324	C23H48	000638-67-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112519\
Data File : BF117995.D
Acq On : 26 Nov 2019 5:01
Operator : JU
Sample : K5840-09 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.09	5.5	ng	190181	1	6.89	694623	20.0
unknown6.66	6.66	31.1	ng	1078580	1	6.89	694623	20.0
n-Hexadecanoic acid	11.96	2.8	ng	98428	4	11.43	695722	20.0
Heneicosane	13.93	5.2	ng	179374	5	14.09	692770	20.0
Tetracosane	14.55	2.4	ng	82548	5	14.09	692770	20.0
Hexacosane	14.86	2.4	ng	61093	6	15.59	514300	20.0
Hexadeca-2,6,10,1...	14.94	2.6	ng	68042	6	15.59	514300	20.0
Docosane, 2,21-di...	15.22	2.9	ng	75149	6	15.59	514300	20.0