

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
 Data File : BF114401.D
 Acq On : 18 May 2019 19:43
 Operator : JU/SJ
 Sample : K2894-18
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-SB-02

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-BF051019.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	25	rVB	5269445	7380578	100.00%	12.171%
2	5.057	502	505	514	rVB	86218	117603	1.59%	0.194%
3	5.469	571	575	592	rVB	3564875	3606260	48.86%	5.947%
4	5.804	630	632	638	rBV	70075	88704	1.20%	0.146%
5	6.481	743	747	758	rBV	2366627	2708348	36.70%	4.466%
6	6.610	765	769	777	rBV	5384767	5477801	74.22%	9.033%
7	6.834	804	807	815	rBV	1791588	1561470	21.16%	2.575%
8	6.992	830	834	841	rBV	5215939	4891601	66.28%	8.066%
9	7.228	868	874	892	rBV4	56720	180251	2.44%	0.297%
10	7.398	893	903	906	rBV	4005376	4400785	59.63%	7.257%
11	7.604	933	938	942	rVB3	56792	77443	1.05%	0.128%
12	7.869	978	983	988	rBV4	221831	330639	4.48%	0.545%
13	8.116	1021	1025	1031	rBV	2137375	1951128	26.44%	3.217%
14	8.175	1031	1035	1038	rVB2	159070	162930	2.21%	0.269%
15	8.404	1071	1074	1079	rVB5	98611	96913	1.31%	0.160%
16	8.481	1081	1087	1092	rBV	512715	757224	10.26%	1.249%
17	8.804	1139	1142	1145	rVB3	123251	127759	1.73%	0.211%
18	8.986	1171	1173	1175	rBV2	90533	91211	1.24%	0.150%
19	9.033	1180	1181	1184	rVB	178961	117229	1.59%	0.193%
20	9.110	1191	1194	1196	rBV	90437	79609	1.08%	0.131%
21	9.133	1196	1198	1202	rVB5	120322	130677	1.77%	0.215%
22	9.192	1202	1208	1211	rBV	6596024	7010275	94.98%	11.560%
23	9.275	1218	1222	1225	rBV3	134078	211940	2.87%	0.349%
24	9.457	1251	1253	1256	rBV2	91619	87863	1.19%	0.145%
25	9.545	1266	1268	1271	rVB2	136777	105151	1.42%	0.173%
26	9.586	1271	1275	1278	rBV4	439274	623328	8.45%	1.028%
27	9.616	1278	1280	1282	rBV2	123499	93958	1.27%	0.155%
28	9.775	1303	1307	1310	rBV4	175081	219570	2.97%	0.362%
29	9.839	1315	1318	1319	rBV	223981	236192	3.20%	0.389%
30	9.869	1319	1323	1327	rVB	2189456	2077192	28.14%	3.425%
31	9.904	1327	1329	1331	rBV2	121961	107184	1.45%	0.177%
32	9.969	1337	1340	1343	rBV3	185269	196358	2.66%	0.324%
33	10.128	1362	1367	1374	rVB3	443895	629110	8.52%	1.037%
34	10.186	1374	1377	1381	rBV4	274754	393307	5.33%	0.649%

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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-BF051019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.351	1403	1405	1410	rVB3	267140	286547	3.88%	0.473%
36	10.510	1429	1432	1436	rVB2	230275	332674	4.51%	0.549%
37	10.633	1450	1453	1454	rBV	352117	279416	3.79%	0.461%
38	10.663	1454	1458	1461	rVV	3610972	3514801	47.62%	5.796%
39	11.357	1573	1576	1581	rBV	2155262	2131466	28.88%	3.515%
40	11.880	1663	1665	1670	rVB4	537411	499963	6.77%	0.824%
41	12.939	1841	1845	1848	rBV	4614391	4542582	61.55%	7.491%
42	13.998	2022	2025	2032	rVB	1233580	1326958	17.98%	2.188%
43	15.468	2271	2275	2281	rVB	1069184	1399766	18.97%	2.308%

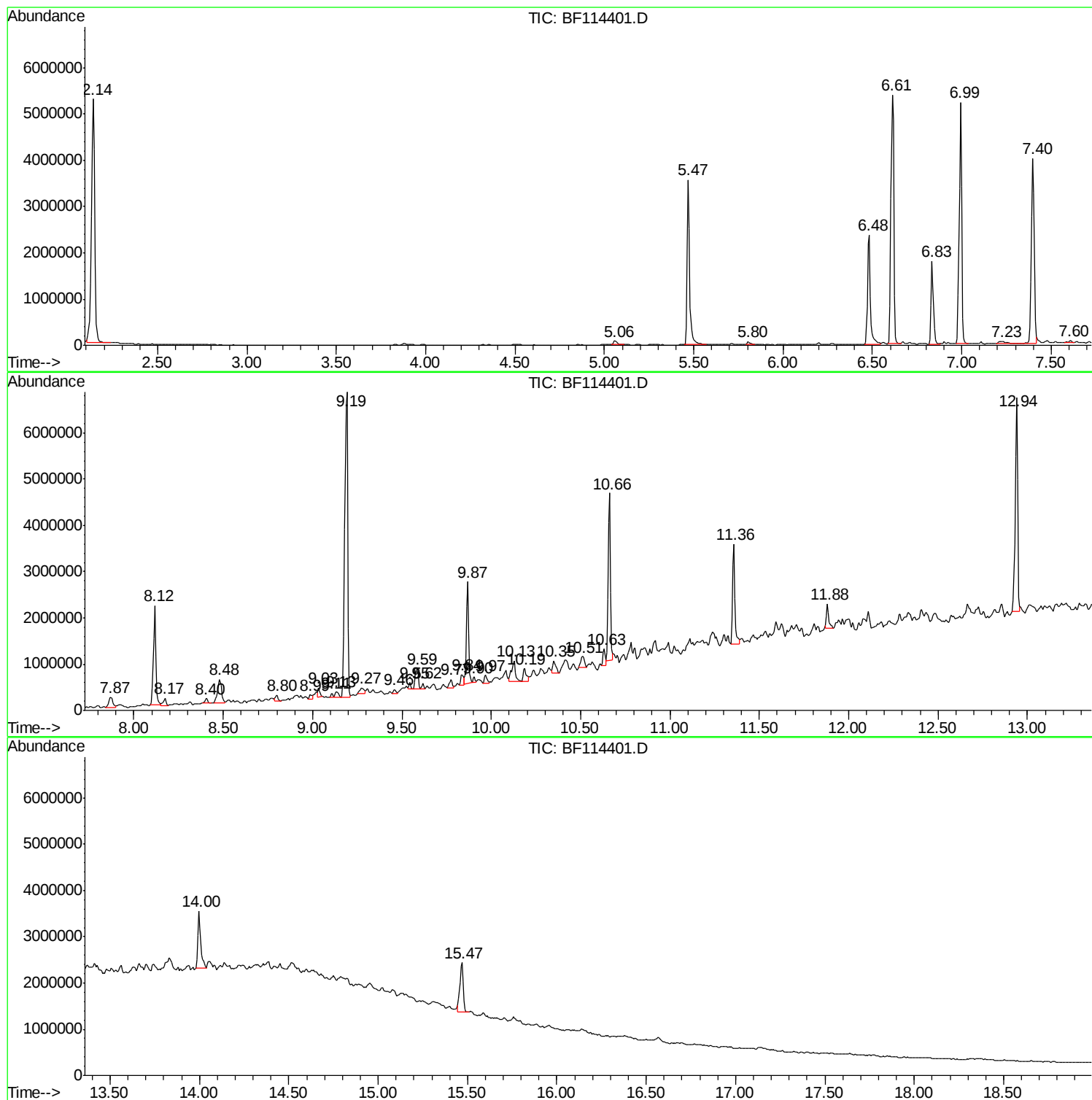
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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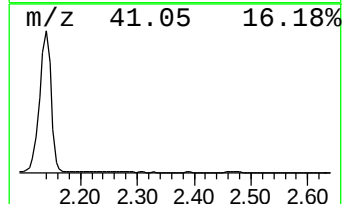
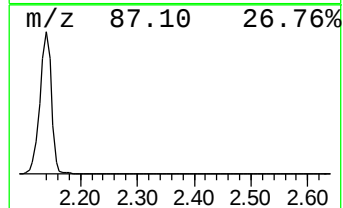
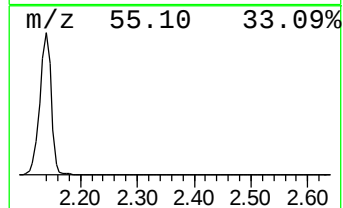
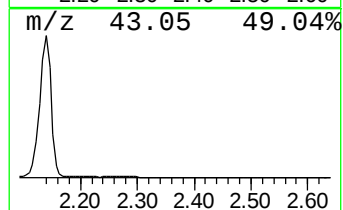
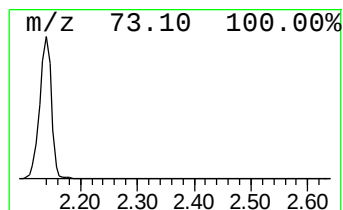
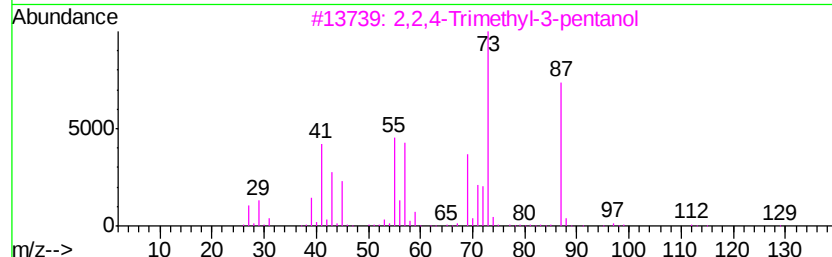
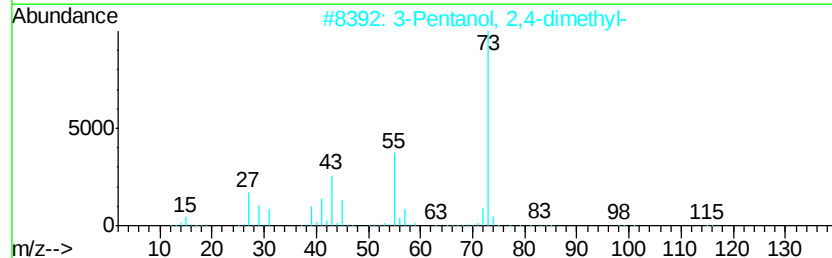
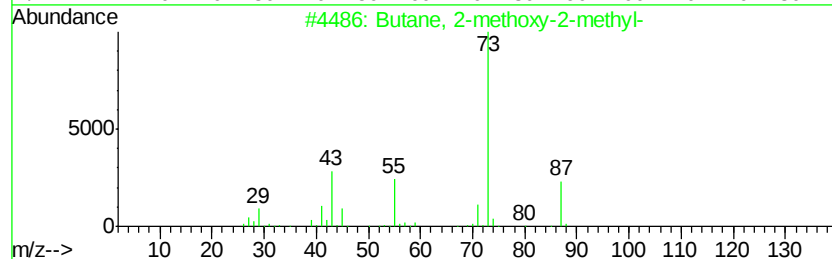
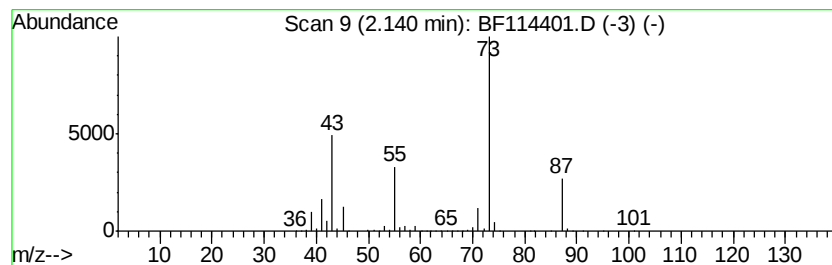
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	94.53 ng	7380580	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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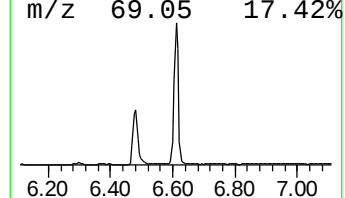
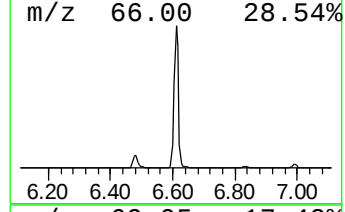
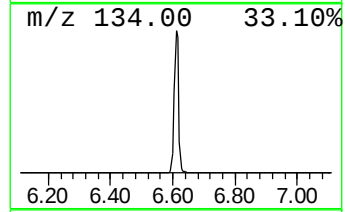
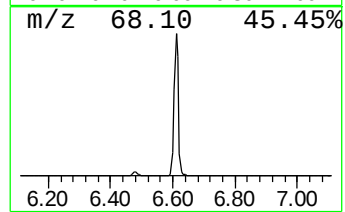
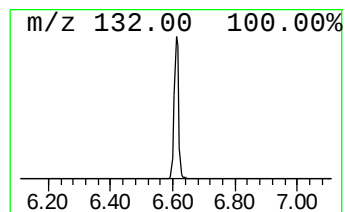
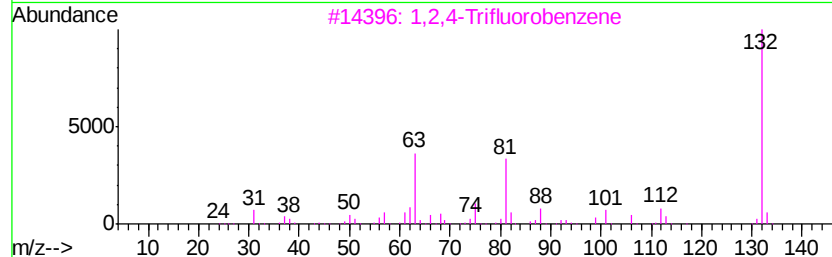
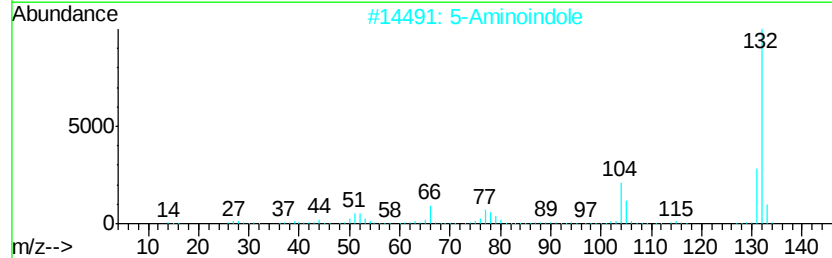
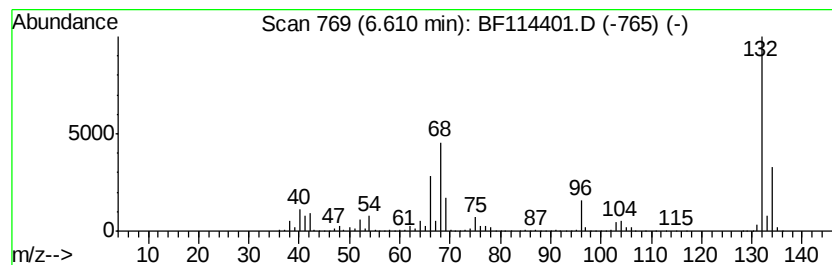
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.61 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	70.16 ng	5477800	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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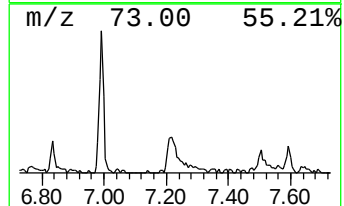
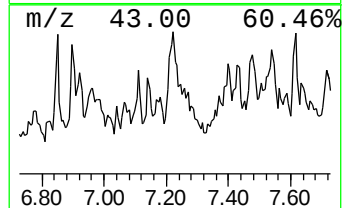
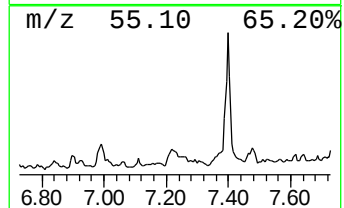
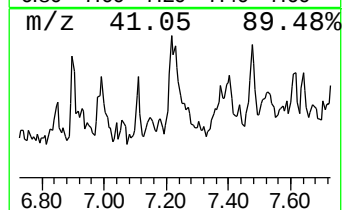
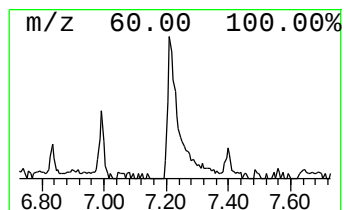
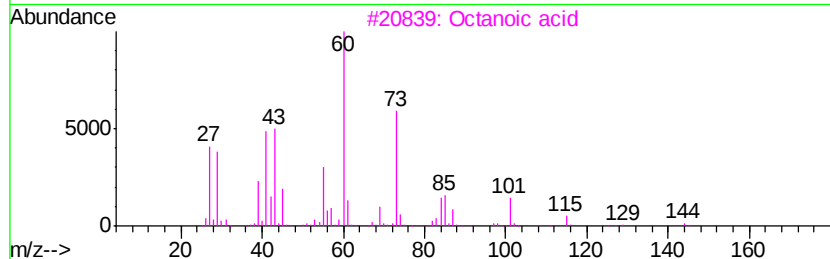
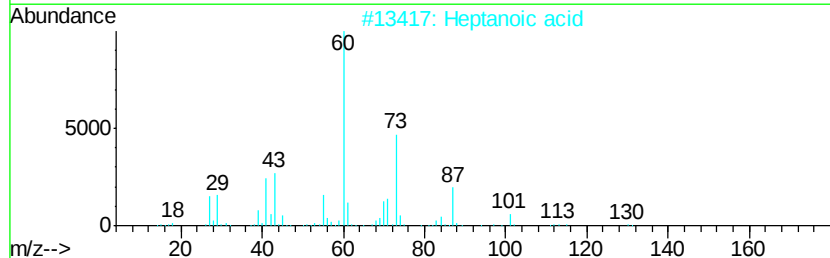
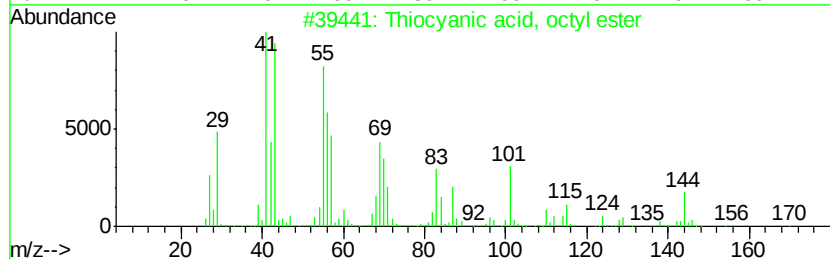
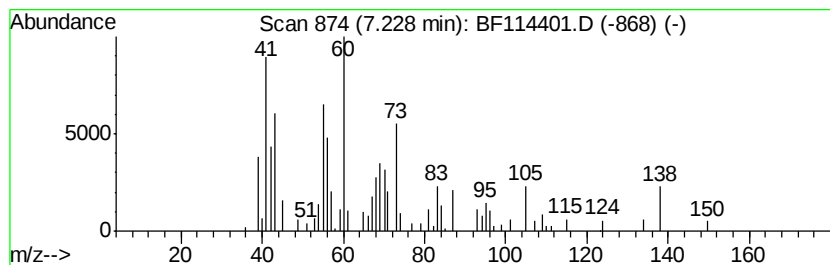
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.23 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	2.31 ng	180251	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiocyanic acid, octyl ester	171	C9H17NS	019942-78-0	35
2		Heptanoic acid	130	C7H14O2	000111-14-8	27
3		Octanoic acid	144	C8H16O2	000124-07-2	22
4		Octane, 2-chloro-	148	C8H17Cl	000628-61-5	16
5		Methyl 10-oxo-8-decenoate	198	C11H18O3	065114-83-2	14



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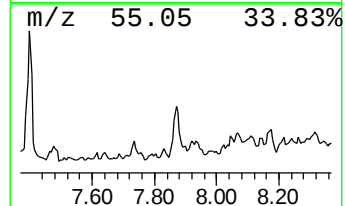
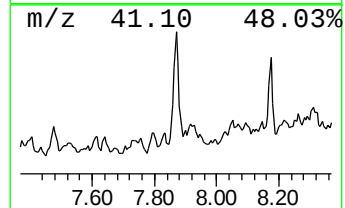
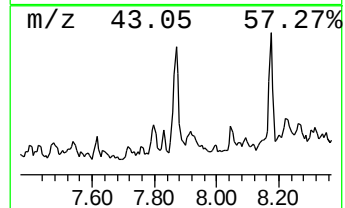
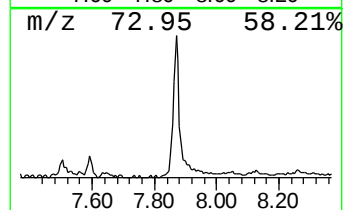
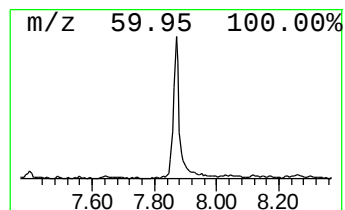
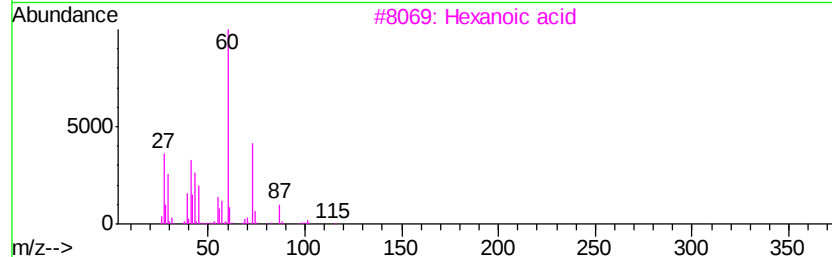
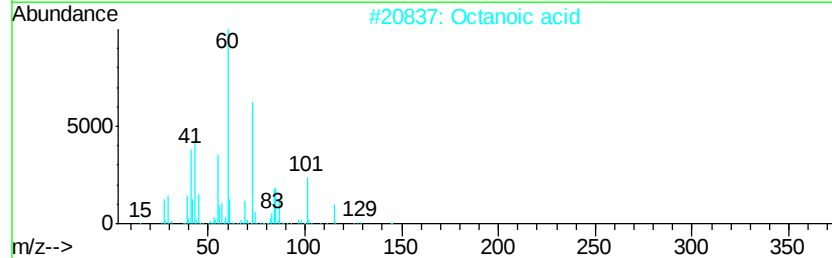
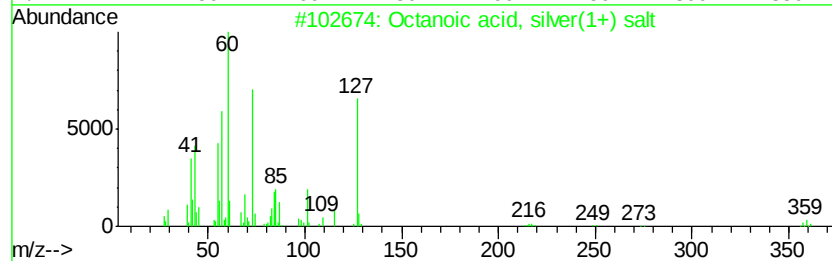
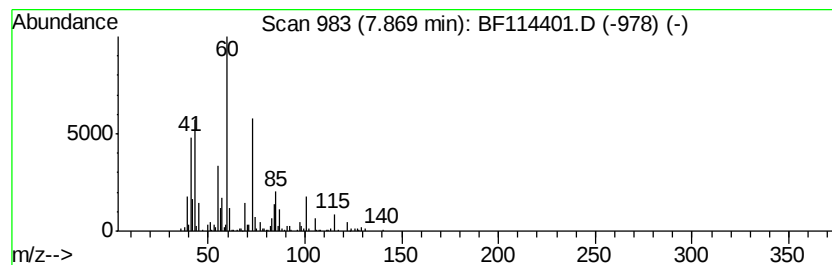
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octanoic acid, silver(1+) salt Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.87	3.39 ng	330639	Napthalene-d8	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	91
2		Octanoic acid	144	C8H16O2	000124-07-2	91
3		Hexanoic acid	116	C6H12O2	000142-62-1	53
4		3-Methyl-hexanoic acid	130	C7H14O2	1000365-65-4	50
5		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	47



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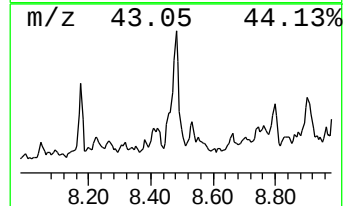
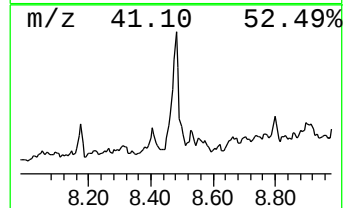
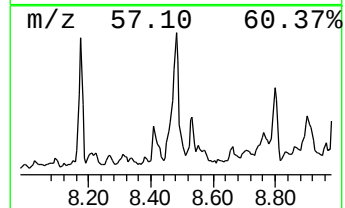
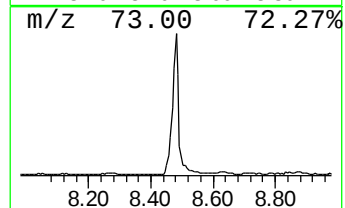
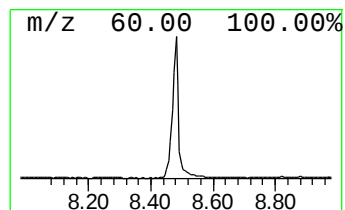
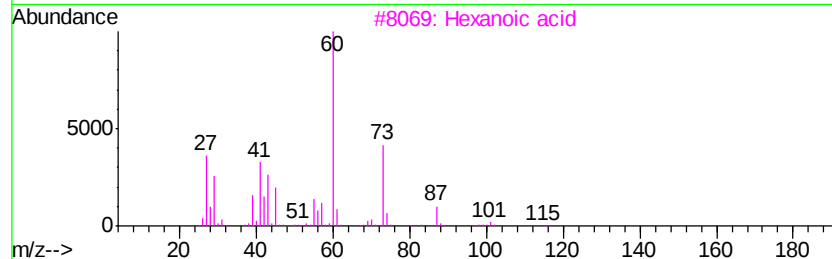
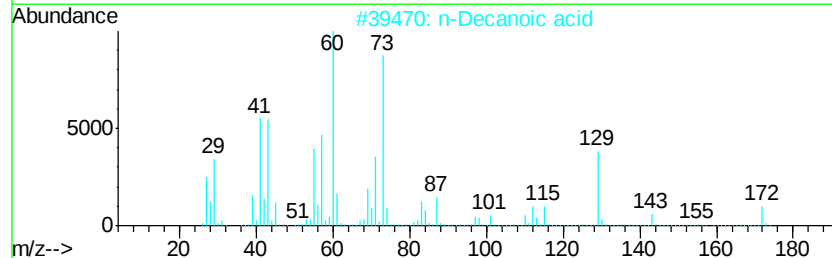
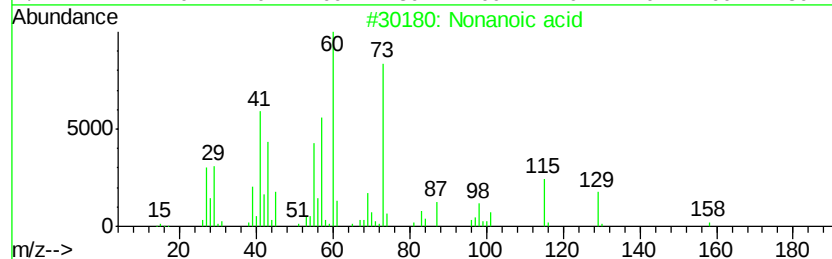
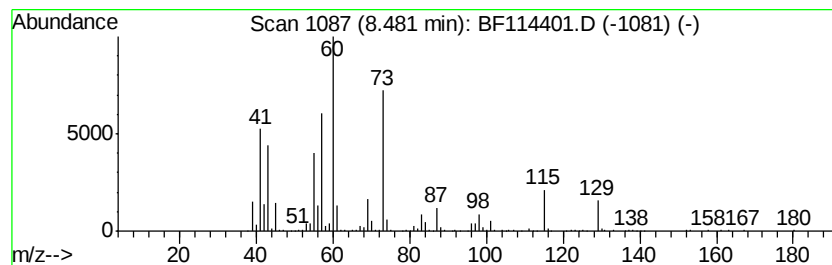
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.48	7.76 ng	757224	Naphthalene-d8	8.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid		158	C9H18O2	000112-05-0	90
2	n-Decanoic acid		172	C10H20O2	000334-48-5	72
3	Hexanoic acid		116	C6H12O2	000142-62-1	59
4	Ethyl .alpha.-d-glucopyranoside		208	C8H16O6	1000127-29-4	59
5	Octanoic acid, silver(1+) salt		250	C8H15AgO2	024927-67-1	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114401.D
Acq On : 18 May 2019 19:43
Operator : JU/SJ
Sample : K2894-18
Misc :
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Instrument :
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ClientSampleId :
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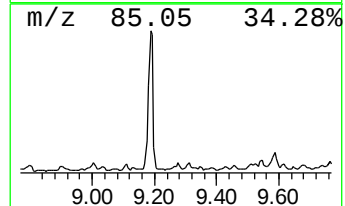
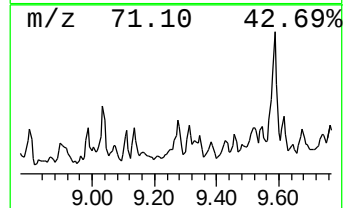
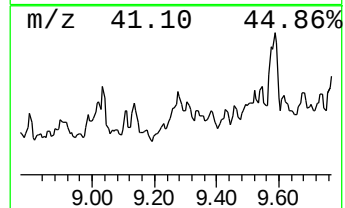
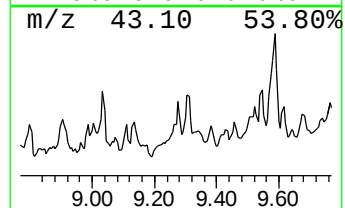
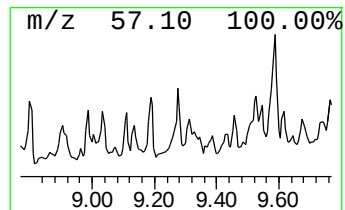
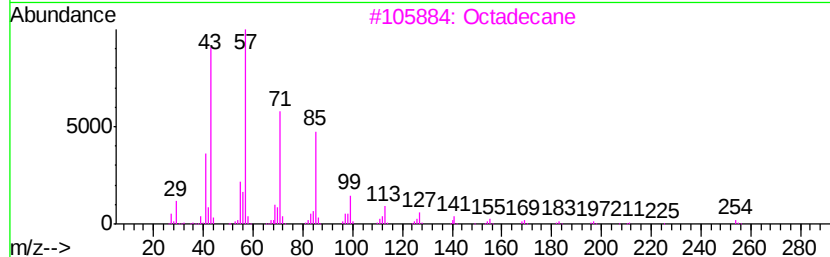
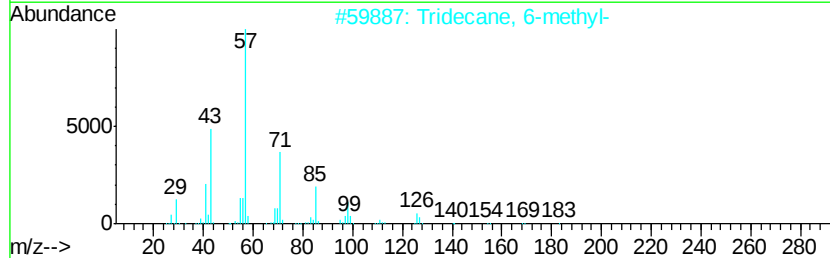
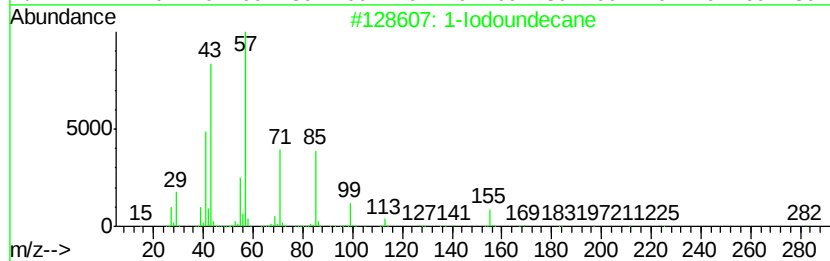
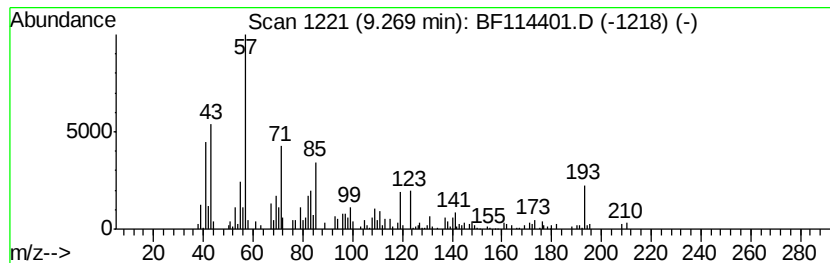
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Iodoundecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	2.04 ng	211940	Acenaphthene-d10	9.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Iodoundecane	282	C11H23I	004282-44-4	52
2		Tridecane, 6-methyl-	198	C14H30	013287-21-3	50
3		Octadecane	254	C18H38	000593-45-3	47
4		Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	47
5		Pentadecane	212	C15H32	000629-62-9	47



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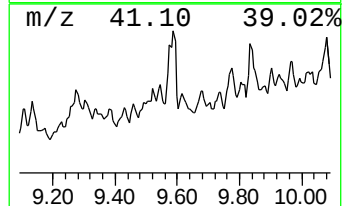
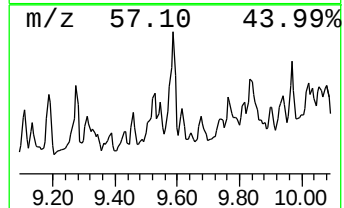
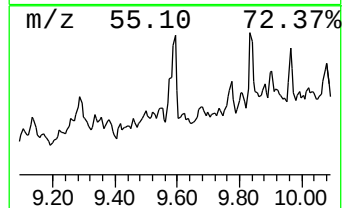
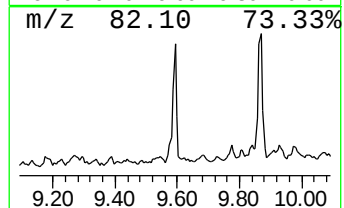
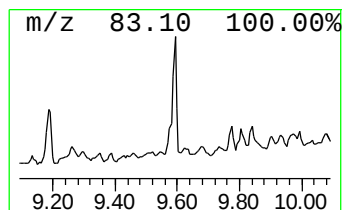
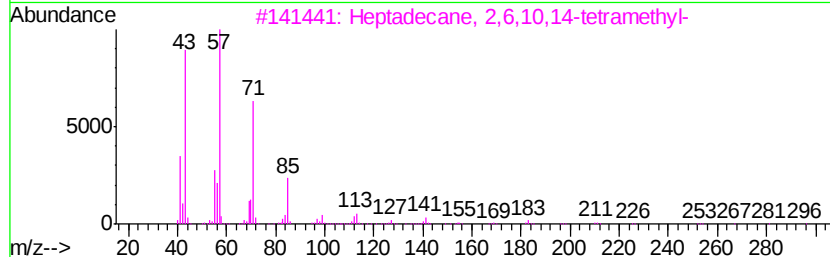
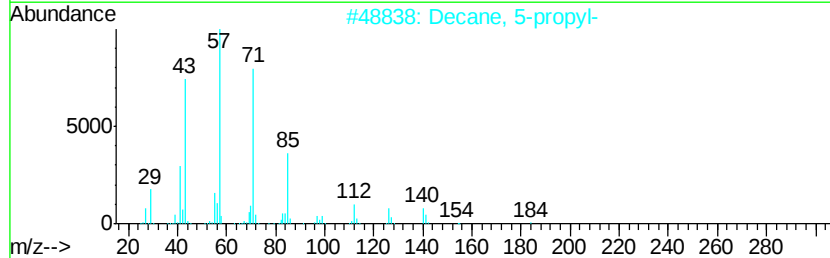
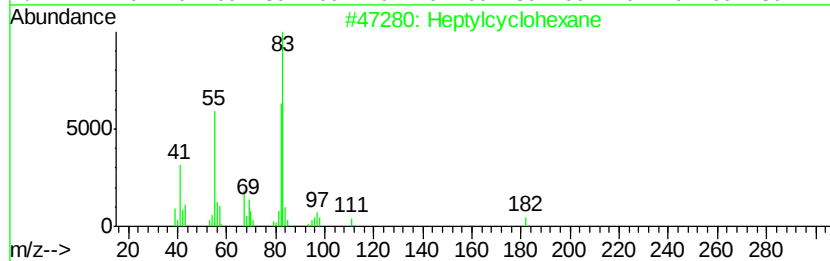
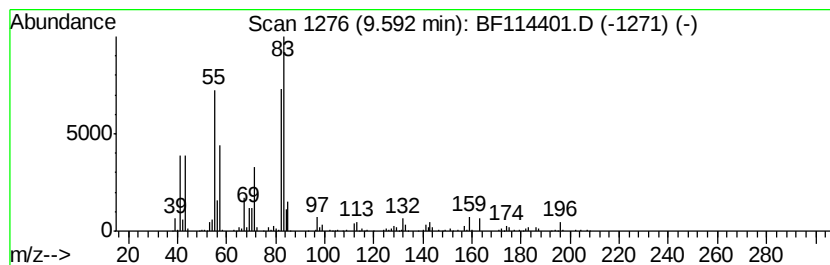
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.59 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.59	6.00 ng	623328	Acenaphthene-d10	9.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptylcyclohexane	182	C13H26	005617-41-4	35
2		Decane, 5-propyl-	184	C13H28	017312-62-8	30
3		Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	30
4		Cyclohexane, pentyl-	154	C11H22	004292-92-6	27
5		Cyclohexane, octyl-	196	C14H28	001795-15-9	27



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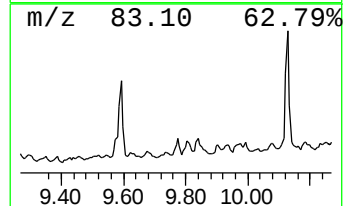
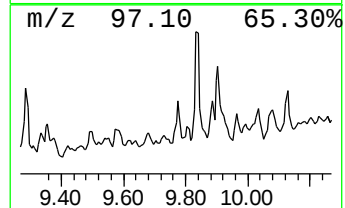
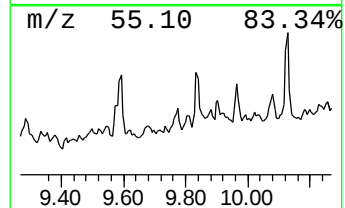
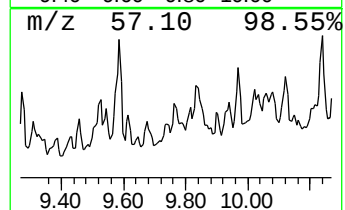
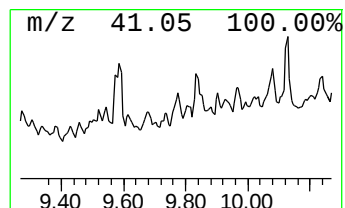
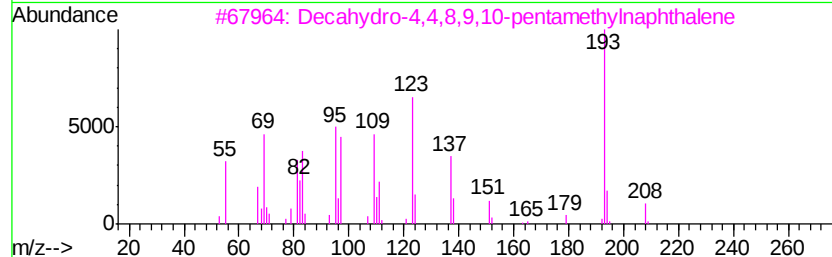
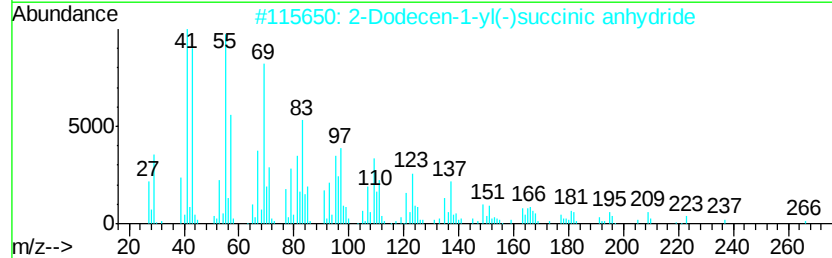
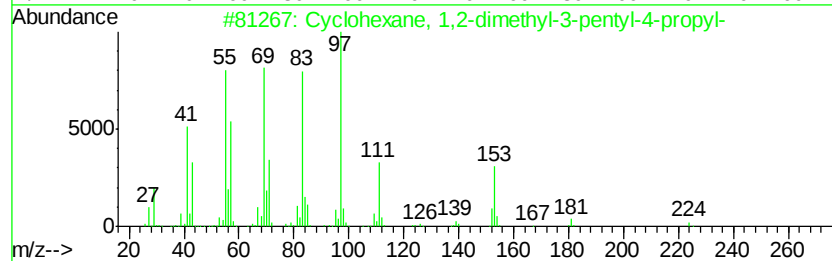
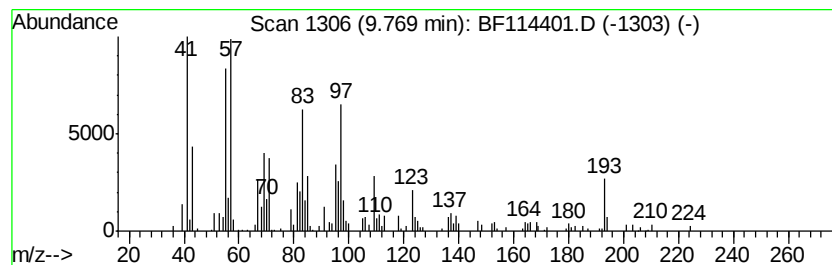
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexane, 1,2-dimethyl-3... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.77	2.11 ng	219570	Acenaphthene-d10	9.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	64
2			2-Dodecen-1-yl(-)succinic anhydride	266	C16H26O3	019780-11-1	53
3			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	38
4			Citronellol	156	C10H20O	000106-22-9	27
5			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
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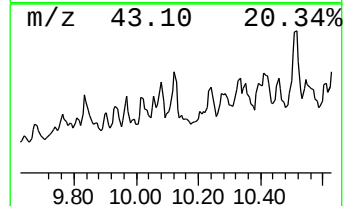
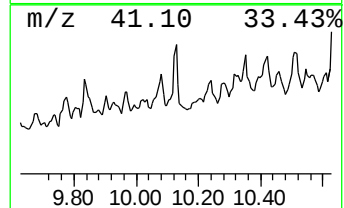
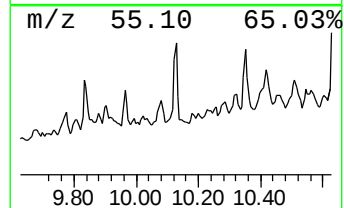
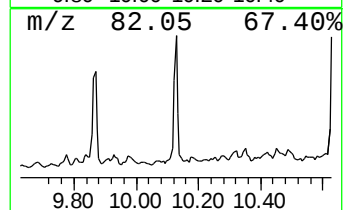
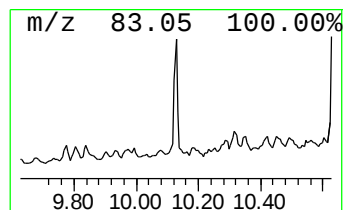
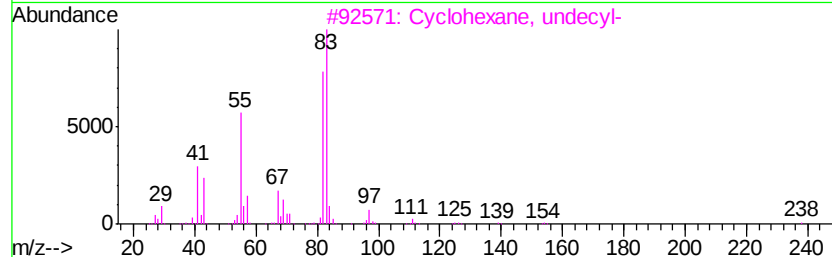
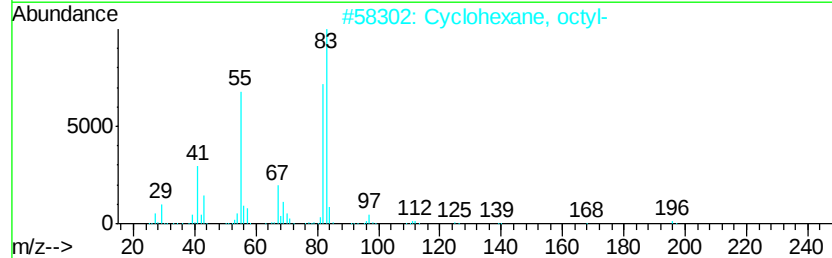
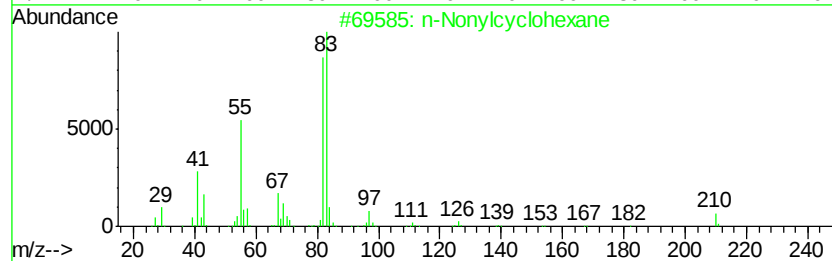
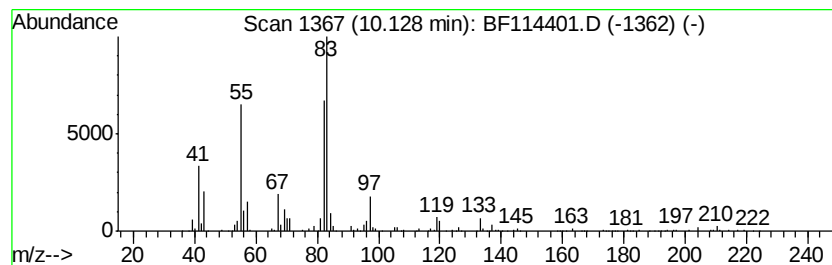
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 n-Nonylcyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.13	6.06 ng	629110	Acenaphthene-d10	9.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Nonylcyclohexane	210	C15H30	002883-02-5	87
2			Cyclohexane, octyl-	196	C14H28	001795-15-9	83
3			Cyclohexane, undecyl-	238	C17H34	054105-66-7	83
4			Cyclohexane, propyl-	126	C9H18	001678-92-8	81
5			Heptylcyclohexane	182	C13H26	005617-41-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
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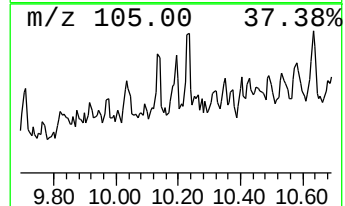
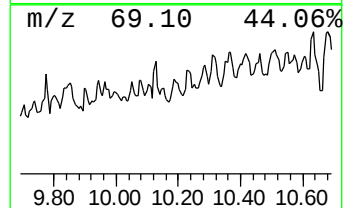
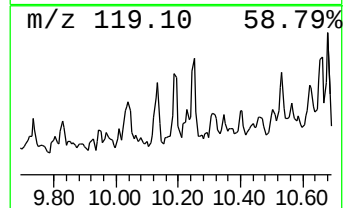
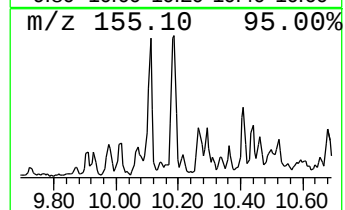
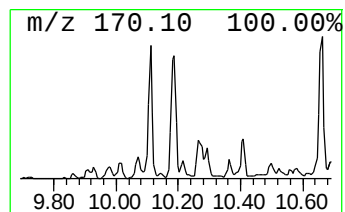
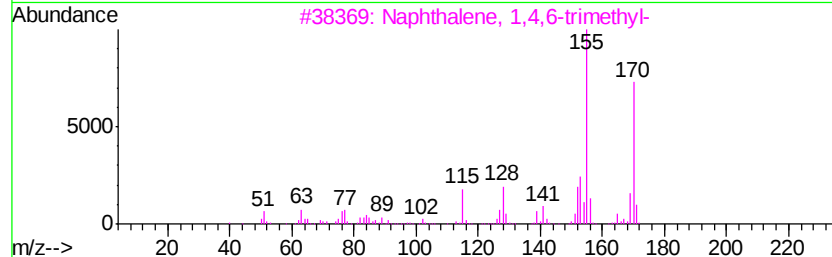
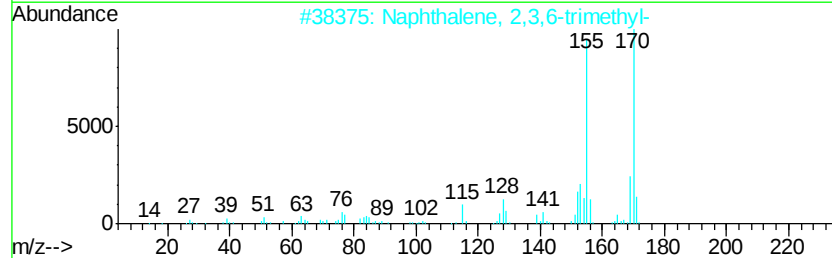
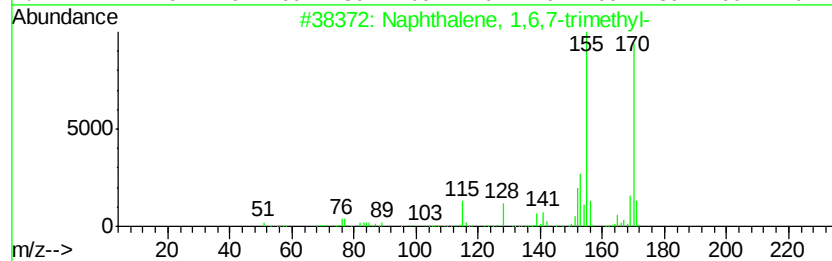
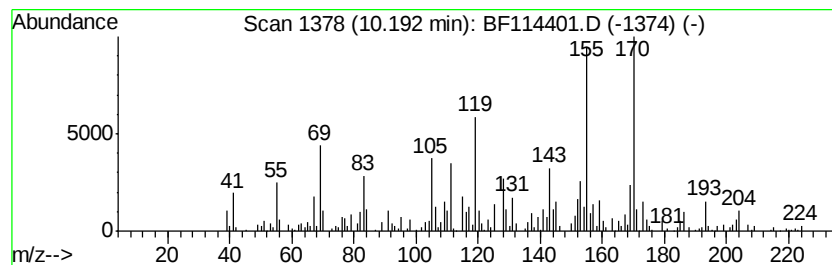
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Naphthalene, 1,6,7-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.19	3.79 ng	393307	Acenaphthene-d10		9.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	96
2	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	96
3	Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	95
4	Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	89
5	4,6,8-Trimethylazulene	170	C13H14	000941-81-1	81



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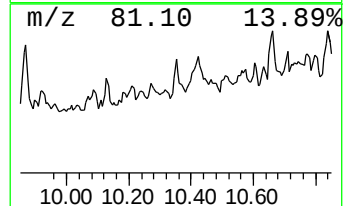
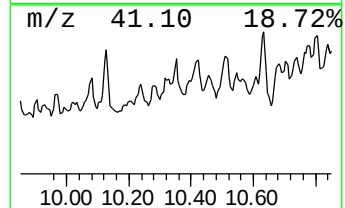
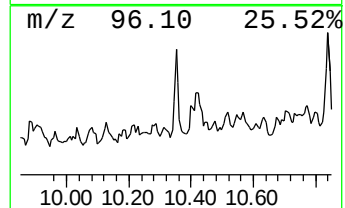
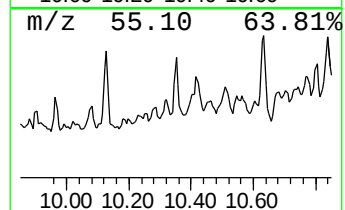
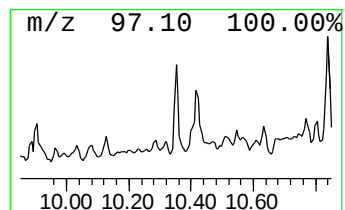
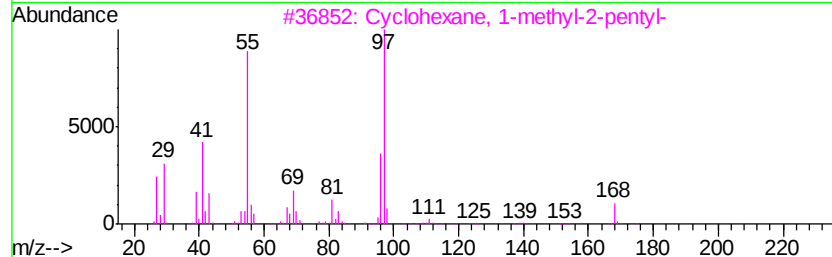
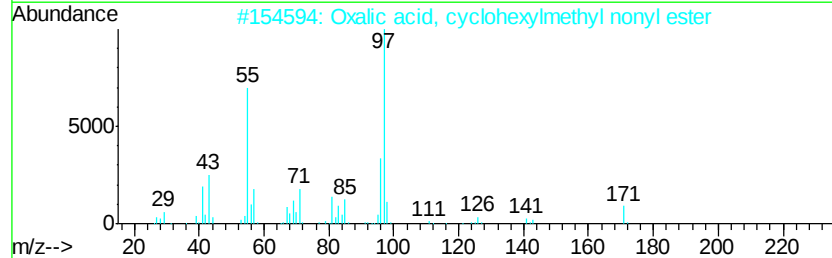
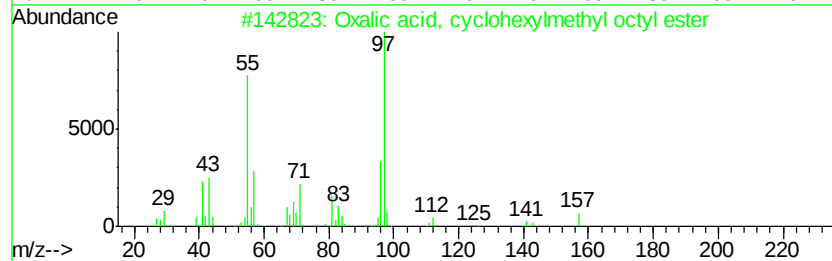
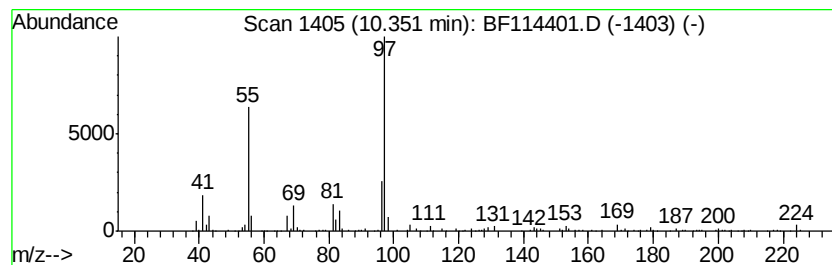
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxalic acid, cyclohexylmeth... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.35	2.76 ng	286547	Acenaphthene-d10	9.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, cyclohexylmethyl oc...	298	C17H30O4	1000309-68-4	86
2			Oxalic acid, cyclohexylmethyl no...	312	C18H32O4	1000309-68-6	78
3			Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	78
4			Trans-1-methyl-2-nonyl-cyclohexane	224	C16H32	1000371-47-8	74
5			Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
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ClientSampleId :
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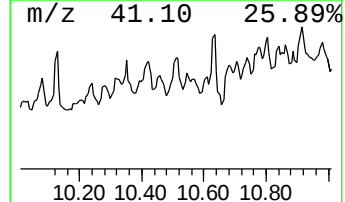
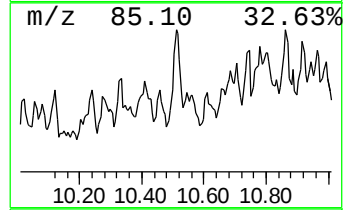
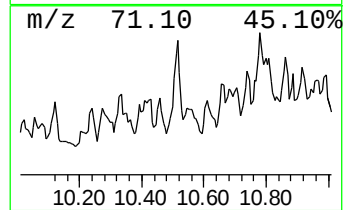
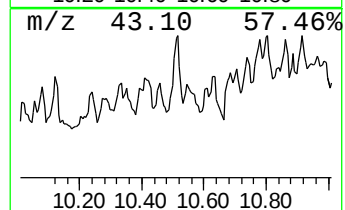
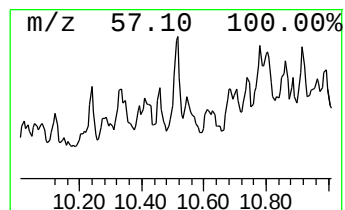
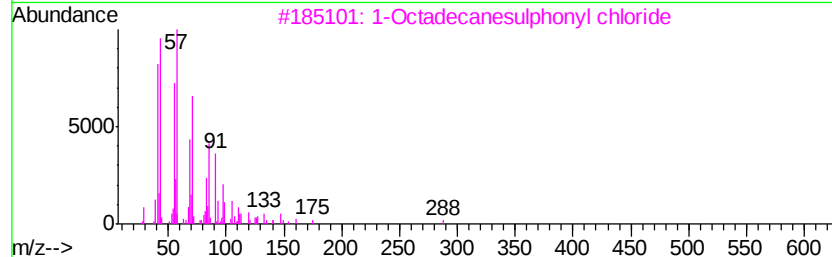
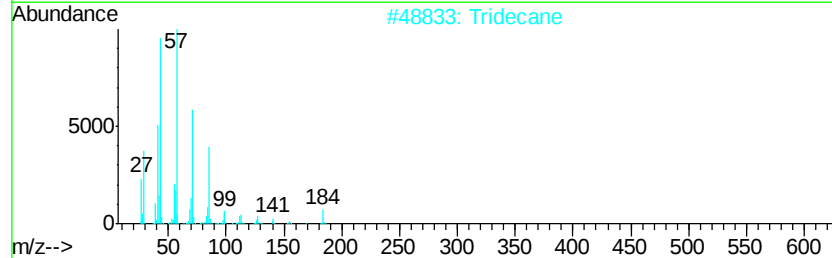
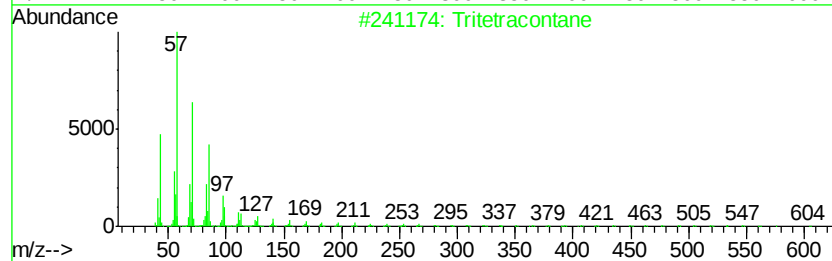
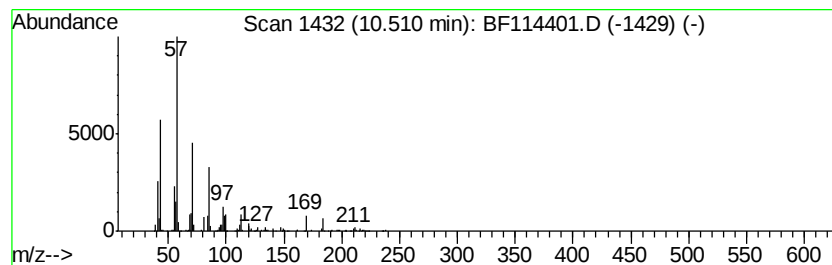
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tritetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	3.20 ng	332674	Acenaphthene-d10	9.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tritetracontane	605	C43H88	007098-21-7	72
2		Tridecane	184	C13H28	000629-50-5	68
3		1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	64
4		Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	58
5		Tetradecane	198	C14H30	000629-59-4	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
Data File : BF114401.D
Acq On : 18 May 2019 19:43
Operator : JU/SJ
Sample : K2894-18
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TWP-SB-02

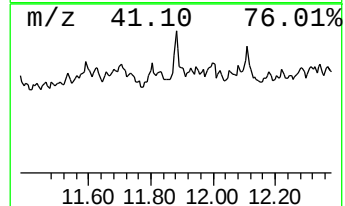
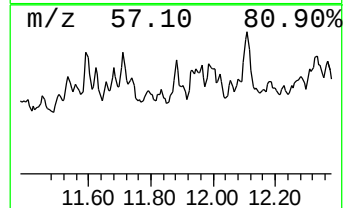
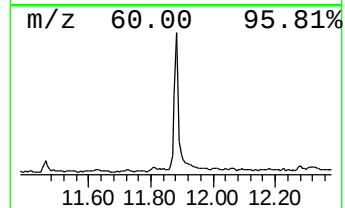
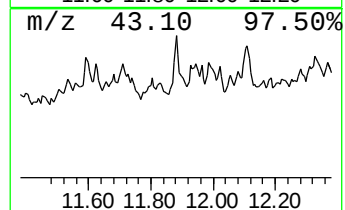
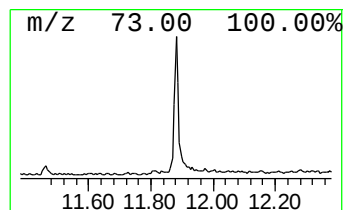
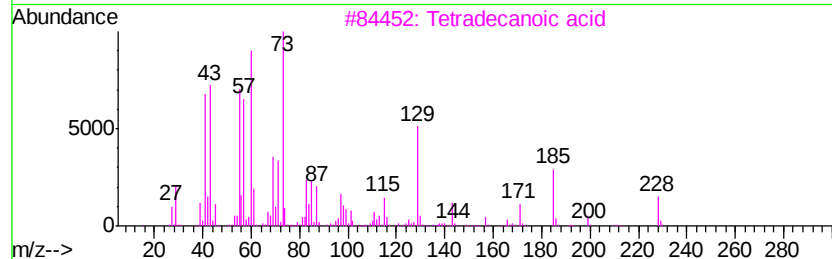
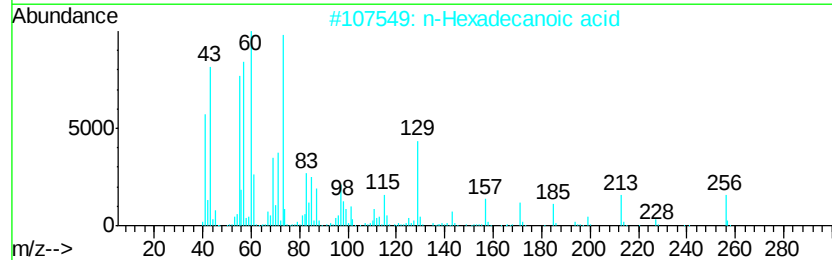
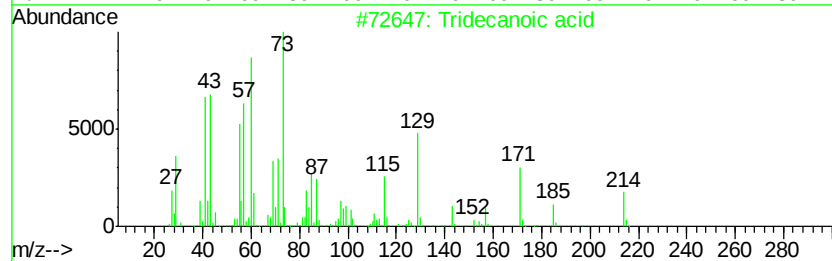
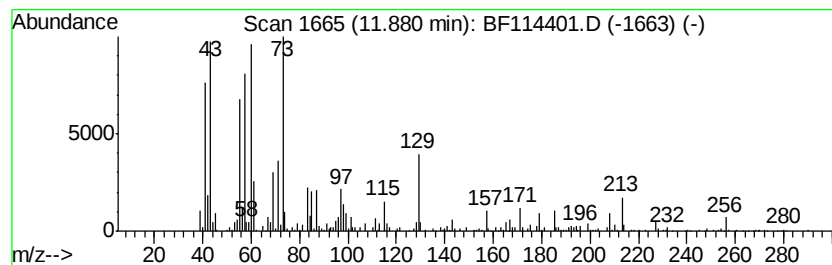
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	4.69 ng	499963	Phenanthrene-d10	11.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051819\
 Data File : BF114401.D
 Acq On : 18 May 2019 19:43
 Operator : JU/SJ
 Sample : K2894-18
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-SB-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051019.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	94.5	ng	7380580	1	6.83	1561470	20.0
unknown6.61	6.61	70.2	ng	5477800	1	6.83	1561470	20.0
unknown7.23	7.23	2.3	ng	180251	1	6.83	1561470	20.0
Octanoic acid, si...	7.87	3.4	ng	330639	2	8.12	1951130	20.0
Nonanoic acid	8.48	7.8	ng	757224	2	8.12	1951130	20.0
1-Iodoundecane	9.27	2.0	ng	211940	3	9.87	2077190	20.0
unknown9.59	9.59	6.0	ng	623328	3	9.87	2077190	20.0
Cyclohexane, 1,2-...	9.77	2.1	ng	219570	3	9.87	2077190	20.0
n-Nonylcyclohexane	10.13	6.1	ng	629110	3	9.87	2077190	20.0
Naphthalene, 1,6,...	10.19	3.8	ng	393307	3	9.87	2077190	20.0
Oxalic acid, cycl...	10.35	2.8	ng	286547	3	9.87	2077190	20.0
Tritetracontane	10.51	3.2	ng	332674	3	9.87	2077190	20.0
Tridecanoic acid	11.88	4.7	ng	499963	4	11.36	2131470	20.0