

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
 Data File : BF096975.D
 Acq On : 22 Jul 2017 7:24
 Operator : SJ/JU
 Sample : I4313-03
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-COMB-1

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:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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	3.352	224	232	242	rBV	70316	131770	2.05%	0.188%
2	3.887	321	323	327	rBV4	30844	89547	1.39%	0.128%
3	3.928	329	330	333	rVB	117805	83965	1.31%	0.120%
4	4.287	362	391	392	rVV3	53773	302102	4.70%	0.431%
5	4.546	434	435	437	rVB	208435	74162	1.15%	0.106%
6	4.716	457	464	472	rBV	143184	176489	2.75%	0.252%
7	5.057	488	522	524	rBV	149353	856448	13.33%	1.223%
8	5.116	529	532	536	rBV3	61065	115132	1.79%	0.164%
9	5.169	538	541	545	rBV	679236	720592	11.22%	1.029%
10	5.346	563	571	572	rBV2	169897	376417	5.86%	0.537%
11	5.428	583	585	587	rVB	382519	270507	4.21%	0.386%
12	5.604	603	615	616	rBV	212703	482117	7.50%	0.688%
13	5.763	640	642	645	rVB	708643	566904	8.82%	0.809%
14	6.051	680	691	692	rBV2	245421	499182	7.77%	0.713%
15	6.193	711	715	717	rVB	420041	492836	7.67%	0.704%
16	6.240	717	723	727	rBV2	816585	1338887	20.84%	1.912%
17	6.334	735	739	743	rBV	1872293	1987593	30.94%	2.838%
18	6.410	744	752	753	rVV3	237624	514901	8.01%	0.735%
19	6.475	761	763	765	rVB	762848	547814	8.53%	0.782%
20	6.557	774	777	781	rVB	954311	784075	12.20%	1.119%
21	6.651	788	793	799	rBV	489434	527127	8.21%	0.753%
22	6.716	799	804	807	rVV	1899340	1787694	27.83%	2.552%
23	6.781	807	815	816	rVV	249092	492991	7.67%	0.704%
24	6.816	816	821	824	rVB	207298	228604	3.56%	0.326%
25	6.851	824	827	828	rBV	59095	65925	1.03%	0.094%
26	6.887	828	833	835	rVB	179918	211731	3.30%	0.302%
27	6.969	843	847	849	rBV	52581	68361	1.06%	0.098%
28	7.010	849	854	857	rVV	3341072	4074369	63.42%	5.817%
29	7.110	857	871	872	rVV	887460	2812274	43.78%	4.015%
30	7.128	872	874	877	rVV	1644411	1245247	19.38%	1.778%
31	7.187	877	884	887	rVV4	87522	167913	2.61%	0.240%
32	7.234	887	892	895	rVV2	58497	78862	1.23%	0.113%
33	7.316	899	906	908	rVV	277192	344097	5.36%	0.491%
34	7.351	908	912	913	rVV4	299631	490355	7.63%	0.700%

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35	7.428	916	925	928	rVV2	388881	896346	13.95%	1.280%
36	7.463	928	931	935	rVV3	118874	159695	2.49%	0.228%
37	7.763	953	982	986	rBV3	1545558	6424378	100.00%	9.172%
38	7.840	992	995	998	rVB	1054032	838184	13.05%	1.197%
39	8.022	1021	1026	1029	rBV4	80389	155781	2.42%	0.222%
40	8.075	1033	1035	1039	rVB2	68635	75176	1.17%	0.107%
41	8.122	1039	1043	1046	rVB2	153081	144663	2.25%	0.207%
42	8.234	1046	1062	1065	rBV	1108486	3163072	49.24%	4.516%
43	8.334	1065	1079	1081	rVV	1540288	3768871	58.67%	5.381%
44	8.375	1083	1086	1090	rVV3	145706	202830	3.16%	0.290%
45	8.410	1090	1092	1097	rVB4	103858	126299	1.97%	0.180%
46	8.492	1102	1106	1111	rVB	714314	644675	10.03%	0.920%
47	8.628	1123	1129	1135	rBV4	104325	229610	3.57%	0.328%
48	8.722	1135	1145	1147	rBV	847492	1650974	25.70%	2.357%
49	8.875	1156	1171	1172	rBV4	1507388	4253411	66.21%	6.073%
50	8.892	1172	1174	1175	rVV	564651	582012	9.06%	0.831%
51	8.916	1175	1178	1187	rVB	2619349	2806491	43.69%	4.007%
52	9.034	1195	1198	1200	rBV	269304	219065	3.41%	0.313%
53	9.151	1213	1218	1222	rVB	306924	326273	5.08%	0.466%
54	9.192	1222	1225	1227	rBV3	76444	96982	1.51%	0.138%
55	9.316	1243	1246	1248	rBV	214765	170884	2.66%	0.244%
56	9.339	1248	1250	1254	rVB	185592	163782	2.55%	0.234%
57	9.416	1259	1263	1265	rVB2	84797	103494	1.61%	0.148%
58	9.463	1269	1271	1276	rVB4	87829	122259	1.90%	0.175%
59	9.528	1278	1282	1287	rBV3	289492	336379	5.24%	0.480%
60	9.586	1287	1292	1299	rVV	968985	983904	15.32%	1.405%
61	9.651	1299	1303	1307	rVB4	112938	154161	2.40%	0.220%
62	9.734	1312	1317	1319	rBV3	168858	278474	4.33%	0.398%
63	9.757	1319	1321	1325	rVB2	165355	172917	2.69%	0.247%
64	9.851	1331	1337	1342	rBV	1134907	1381499	21.50%	1.972%
65	9.992	1356	1361	1363	rBV3	265553	337939	5.26%	0.482%
66	10.086	1374	1377	1382	rVB2	116755	104694	1.63%	0.149%
67	10.175	1387	1392	1397	rBV3	328722	440030	6.85%	0.628%
68	10.257	1403	1406	1408	rBV2	71421	64857	1.01%	0.093%
69	10.286	1408	1411	1412	rVV2	119891	118936	1.85%	0.170%
70	10.310	1412	1415	1417	rVV2	182861	198015	3.08%	0.283%
71	10.333	1417	1419	1422	rVV3	83712	105438	1.64%	0.151%

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72	10.375	1422	1426	1431	rVB	892332	811181	12.63%	1.158%
73	10.457	1436	1440	1444	rBV3	173005	267073	4.16%	0.381%
74	10.510	1444	1449	1453	rBV3	222525	293333	4.57%	0.419%
75	10.569	1457	1459	1461	rBV	157598	124851	1.94%	0.178%
76	10.604	1461	1465	1468	rBV2	238604	281127	4.38%	0.401%
77	10.639	1468	1471	1472	rVV2	140183	133901	2.08%	0.191%
78	10.663	1472	1475	1480	rVB2	151083	172806	2.69%	0.247%
79	10.775	1490	1494	1500	rVB2	739809	845955	13.17%	1.208%
80	10.828	1500	1503	1507	rVB	106817	108471	1.69%	0.155%
81	10.951	1521	1524	1526	rBV2	164966	156791	2.44%	0.224%
82	11.004	1530	1533	1536	rVB2	84900	84723	1.32%	0.121%
83	11.063	1538	1543	1545	rBV	781613	794758	12.37%	1.135%
84	11.204	1564	1567	1572	rBV3	159042	165388	2.57%	0.236%
85	11.257	1572	1576	1579	rVB2	309632	299370	4.66%	0.427%
86	11.351	1590	1592	1595	rVB	136283	110802	1.72%	0.158%
87	11.380	1595	1597	1600	rBV3	89552	102082	1.59%	0.146%
88	11.410	1600	1602	1605	rVV	82113	65846	1.02%	0.094%
89	11.551	1624	1626	1631	rVV4	110829	146458	2.28%	0.209%
90	11.651	1634	1643	1657	rVB	2788198	5146848	80.11%	7.348%
91	11.875	1678	1681	1684	rBV2	70278	86819	1.35%	0.124%
92	12.333	1755	1759	1766	rBV2	362469	726689	11.31%	1.038%
93	12.410	1768	1772	1776	rBV	954217	1104492	17.19%	1.577%
94	12.645	1809	1812	1816	rBV	1292063	1277915	19.89%	1.825%
95	13.233	1909	1912	1915	rVB	326607	324098	5.04%	0.463%
96	13.692	1986	1990	1993	rBV	698092	674093	10.49%	0.962%
97	14.339	2097	2100	2104	rBV	196537	204663	3.19%	0.292%
98	15.057	2218	2222	2226	rVB	470262	520502	8.10%	0.743%

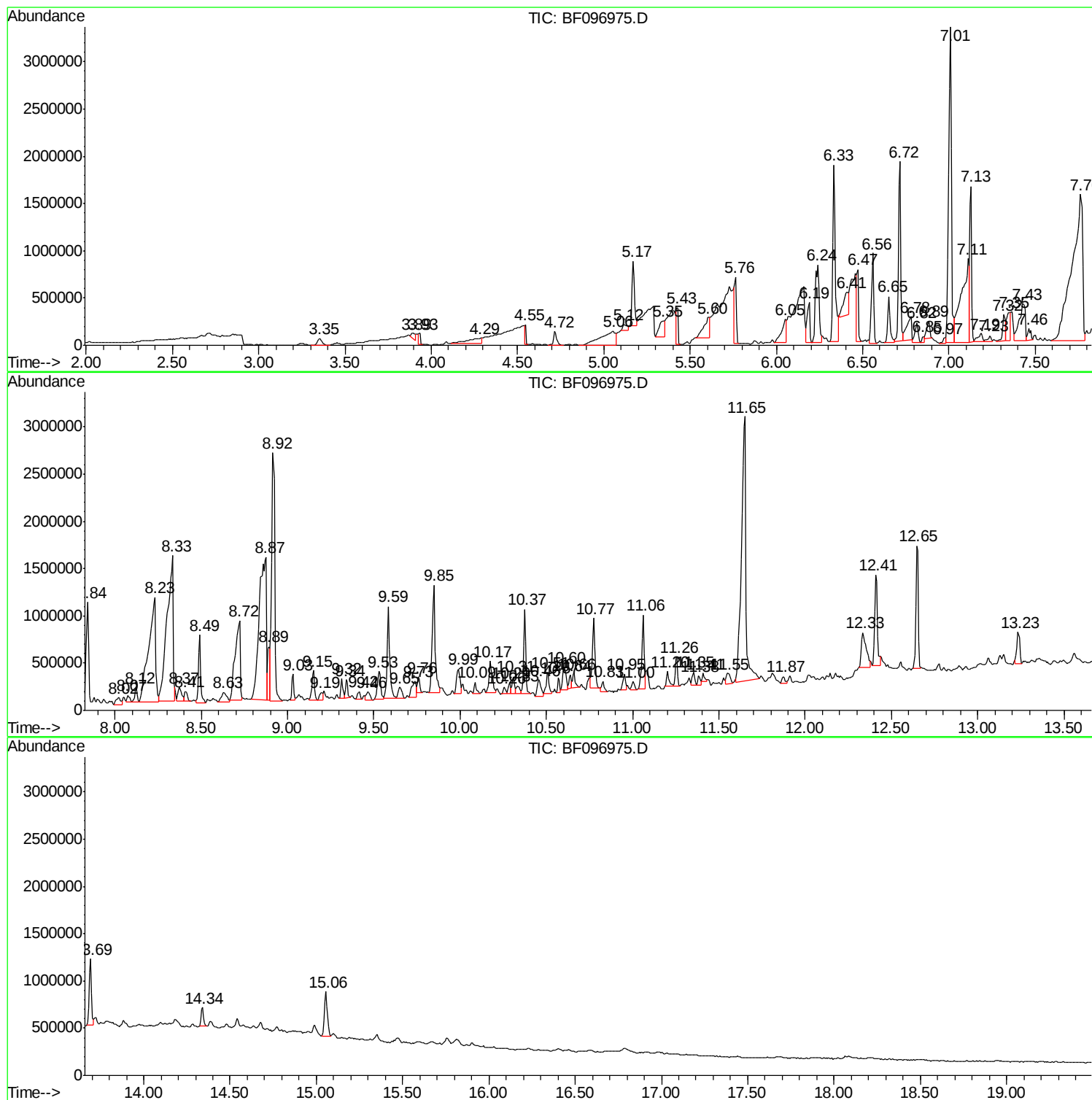
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Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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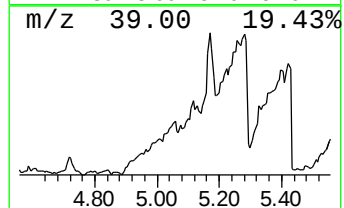
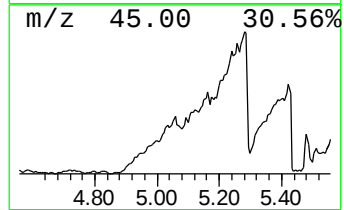
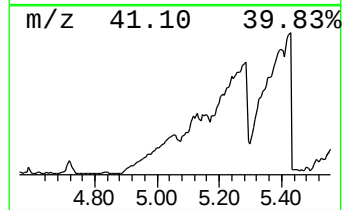
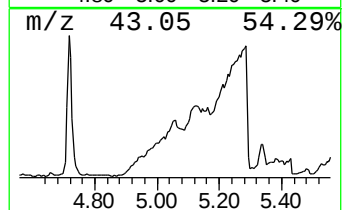
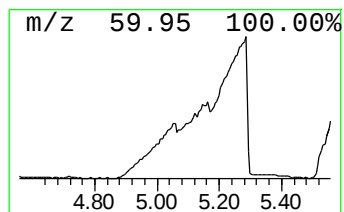
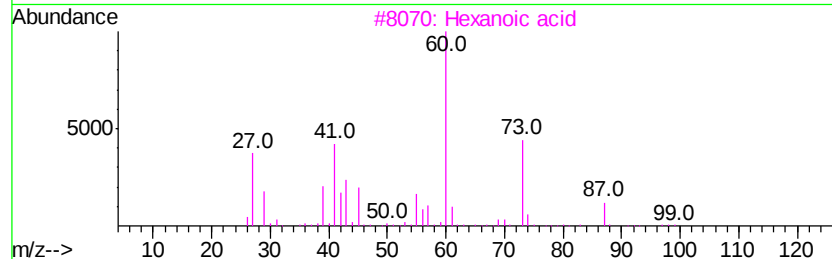
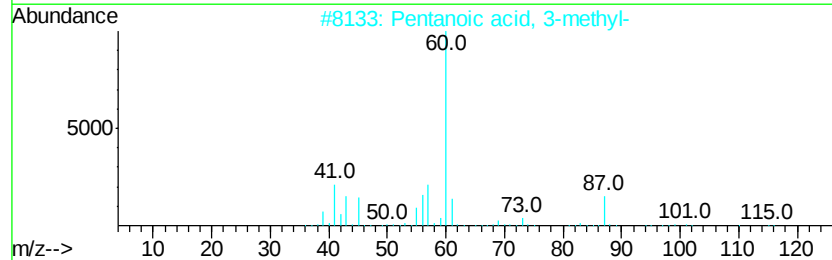
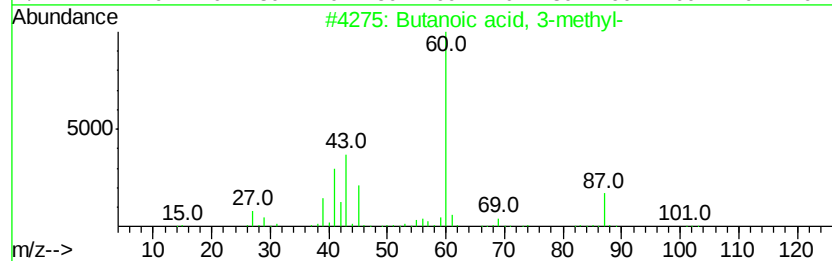
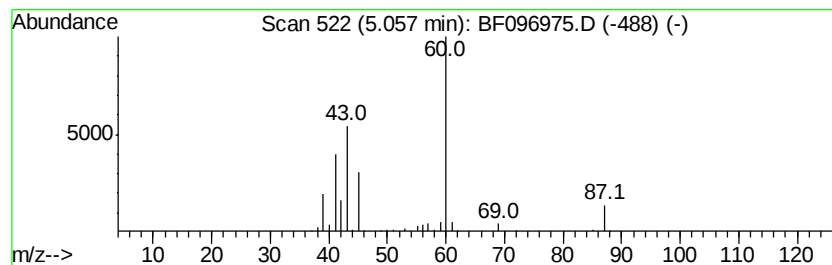
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	21.85 ng	856448	1,4-Dichlorobenzene-d4	6.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	83
2		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	56
3		Hexanoic acid	116	C6H12O2	000142-62-1	39
4		1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	39
5		Formic acid hydrazide	60	CH4N2O	000624-84-0	9



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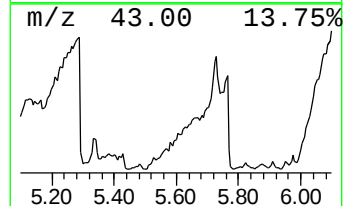
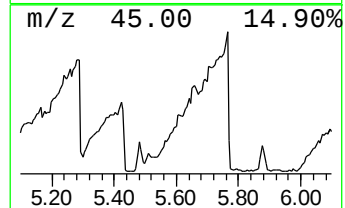
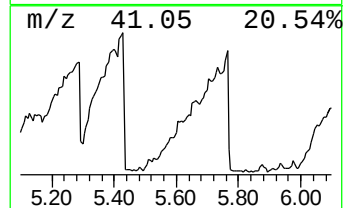
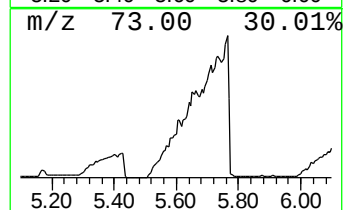
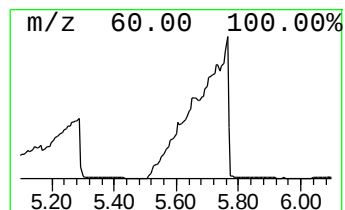
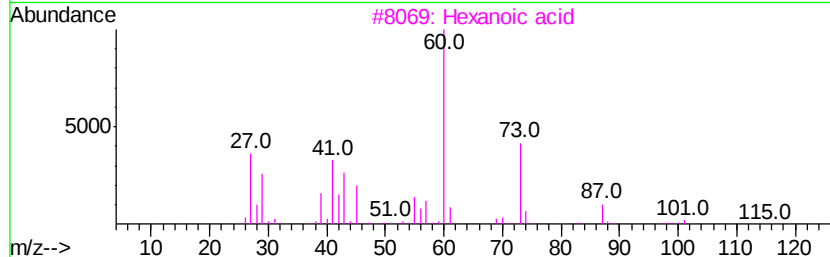
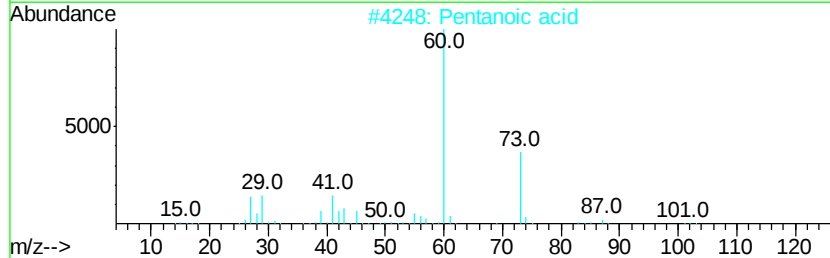
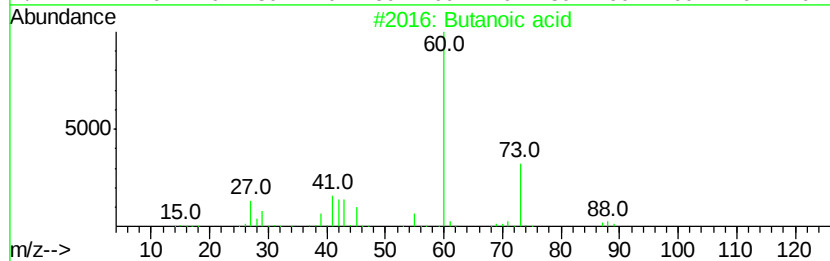
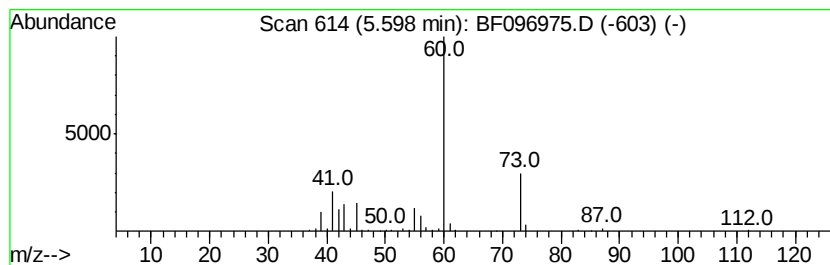
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	12.30 ng	482117	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	78
2		Pentanoic acid	102	C5H10O2	000109-52-4	78
3		Hexanoic acid	116	C6H12O2	000142-62-1	78
4		.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	40
5		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	38



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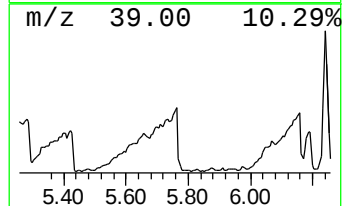
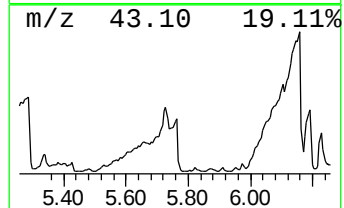
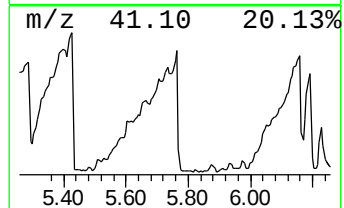
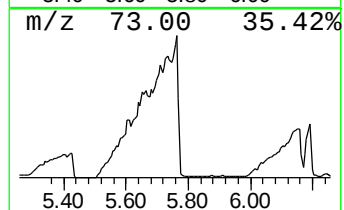
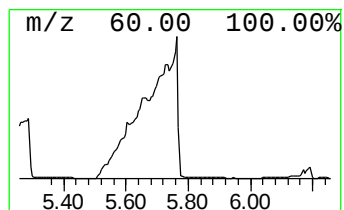
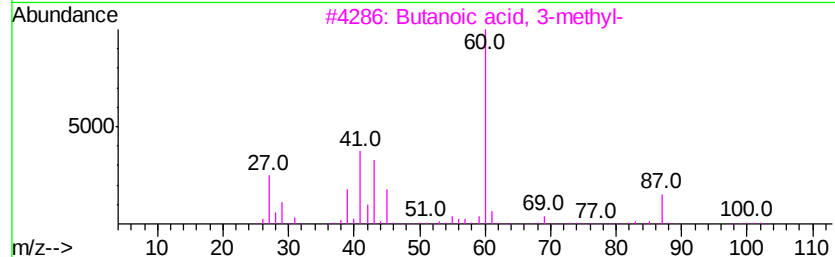
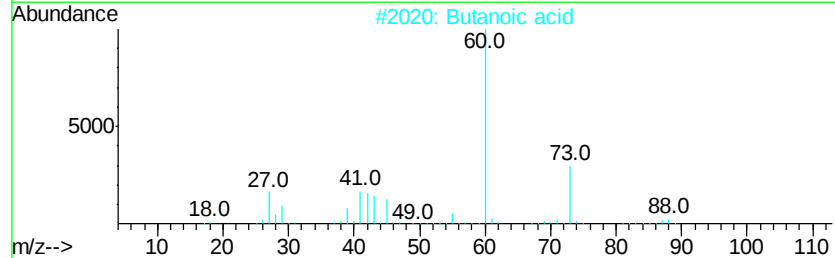
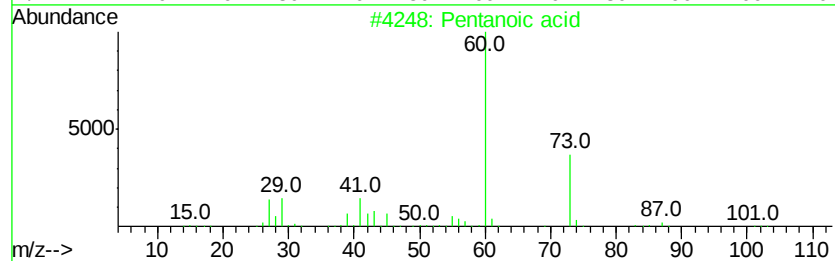
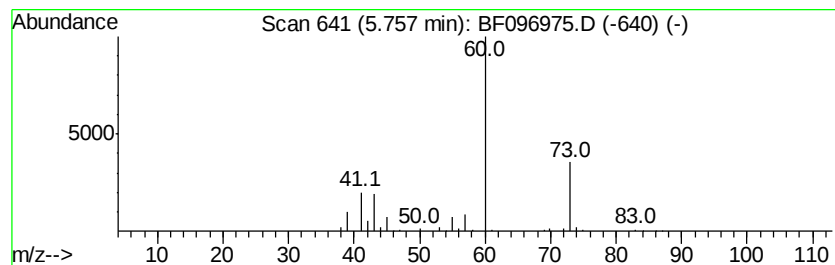
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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Peak Number 3 Pentanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.76	14.46 ng	566904	1,4-Dichlorobenzene-d4	6.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentanoic acid	102	C5H10O2	000109-52-4	74
2		Butanoic acid	88	C4H8O2	000107-92-6	72
3		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
4		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	42
5		Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096975.D
Acq On : 22 Jul 2017 7:24
Operator : SJ/JU
Sample : I4313-03
Misc :
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ClientSampleId :
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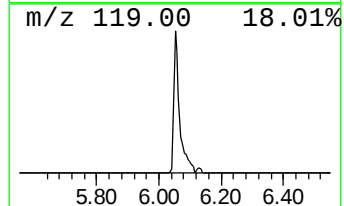
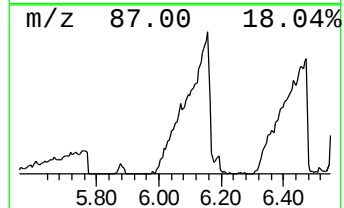
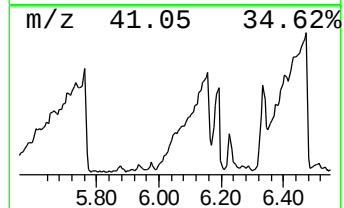
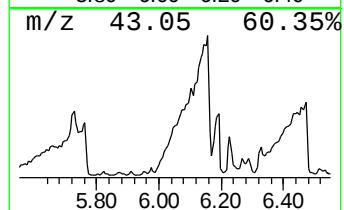
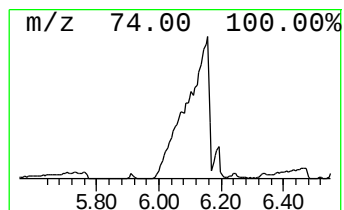
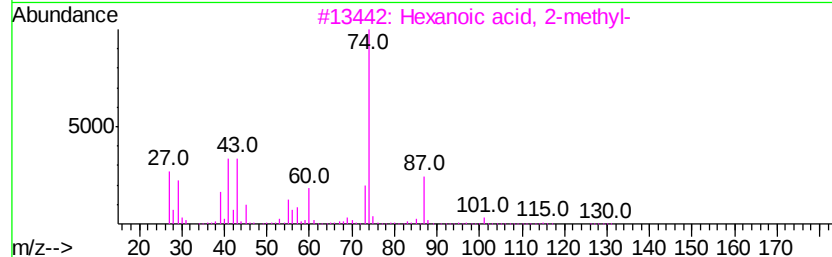
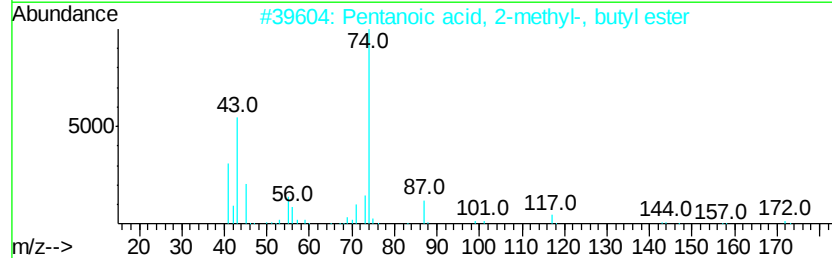
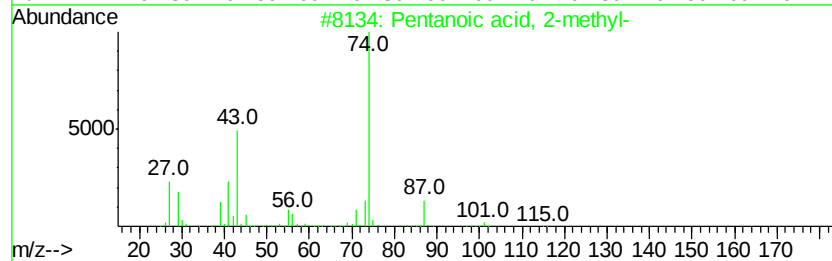
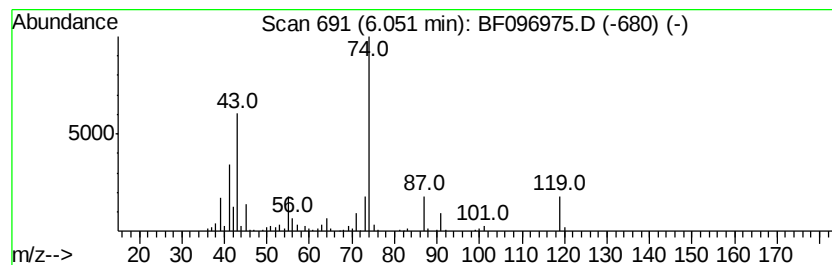
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Pentanoic acid, 2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.05	12.73 ng	499182	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	59
2		Pentanoic acid, 2-methyl-, butyl...	172	C10H20O2	006297-41-2	45
3		Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	42
4		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	33
5		Ethanol, 2-[(2-aminoethyl)amino]-	104	C4H12N2O	000111-41-1	28



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096975.D
Acq On : 22 Jul 2017 7:24
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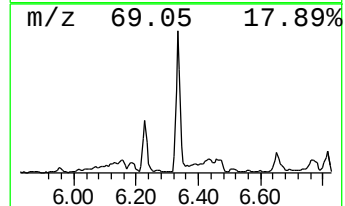
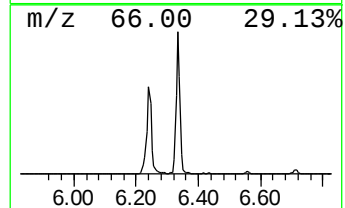
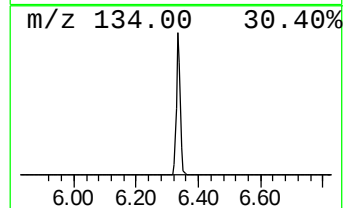
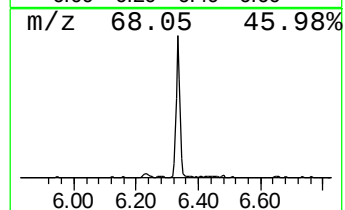
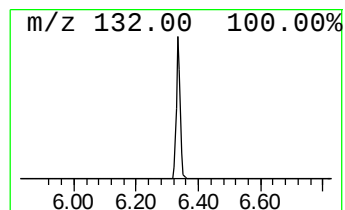
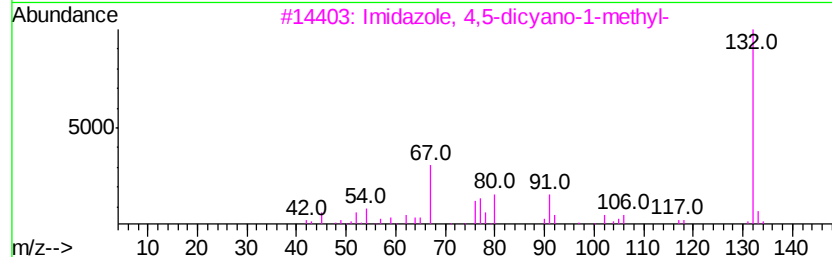
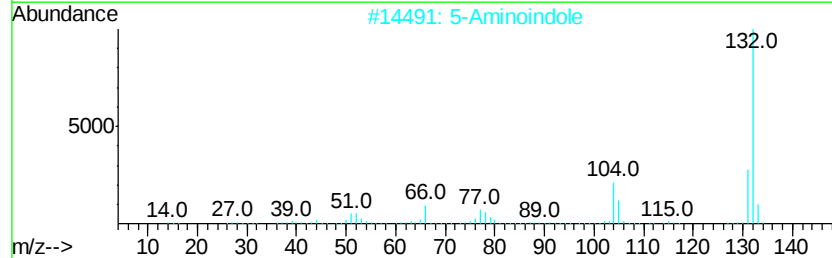
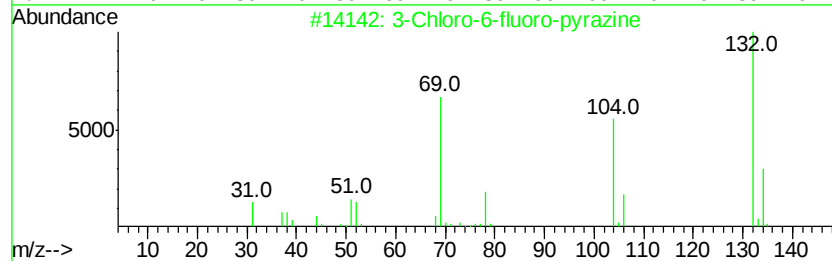
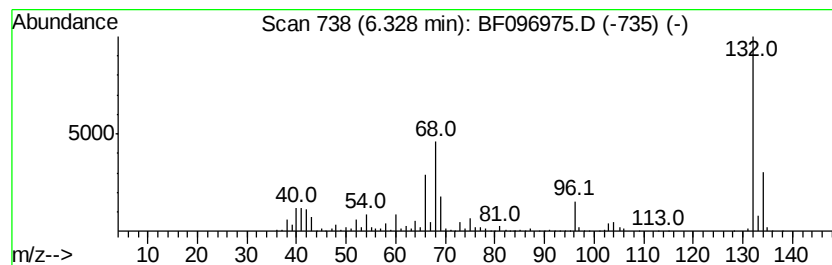
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.33 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	50.70 ng	1987590	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	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	



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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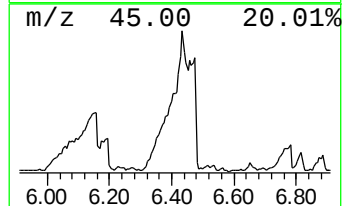
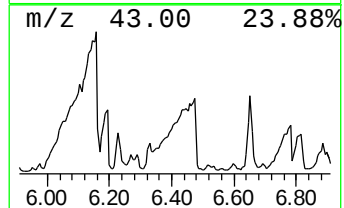
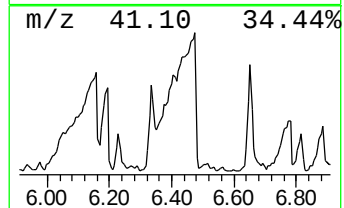
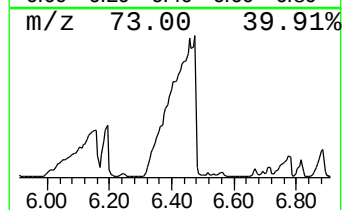
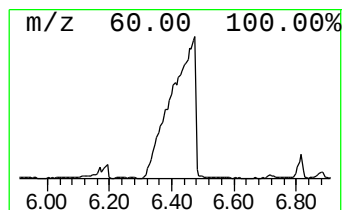
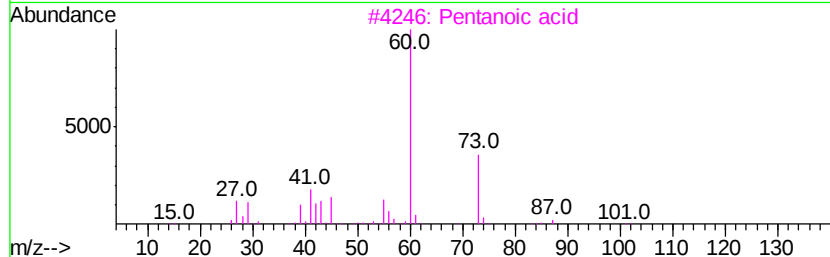
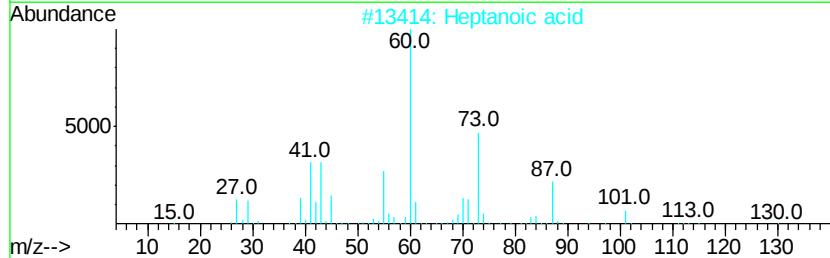
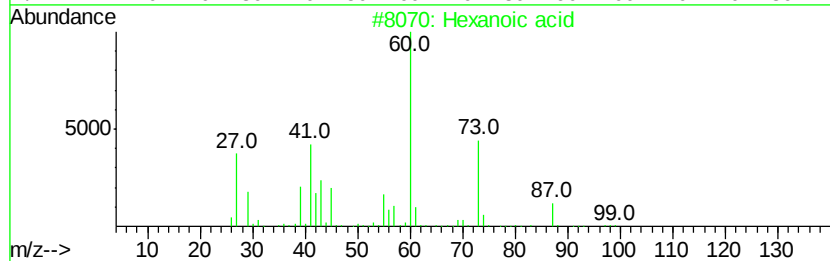
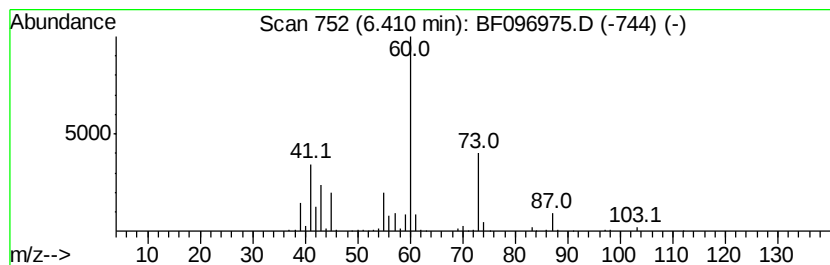
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanoic acid Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	13.13 ng	514901	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid	116	C6H12O2	000142-62-1	90
2		Heptanoic acid	130	C7H14O2	000111-14-8	72
3		Pentanoic acid	102	C5H10O2	000109-52-4	72
4		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
5		D-Fucose	164	C6H12O5	003615-37-0	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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Operator : SJ/JU
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ClientSampleId :
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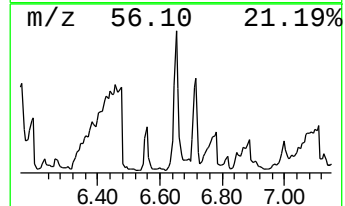
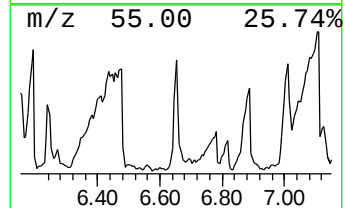
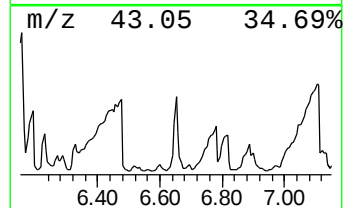
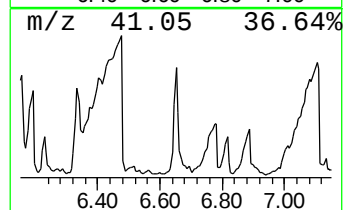
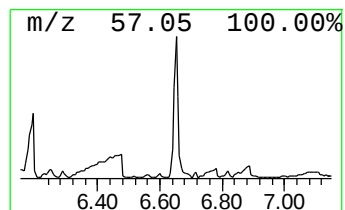
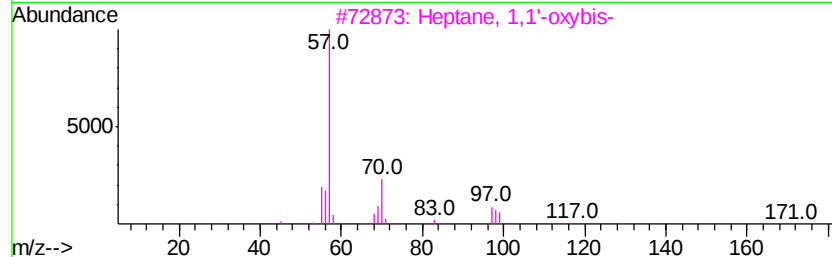
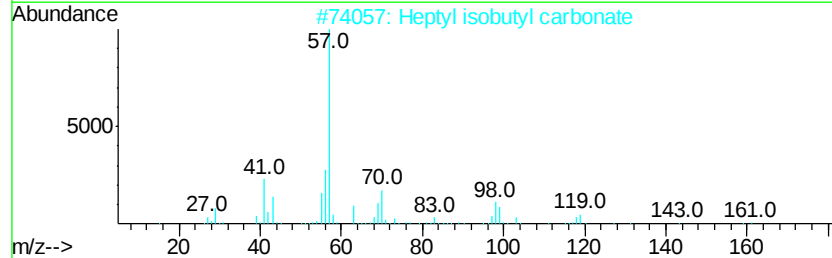
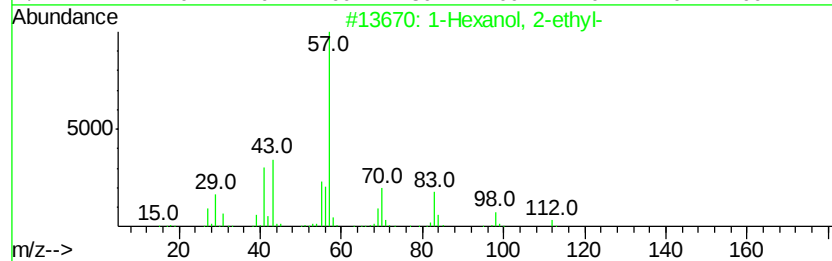
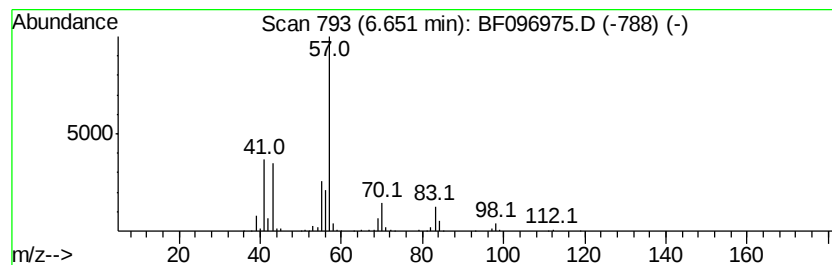
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	13.45 ng	527127	1,4-Dichlorobenzene-d4	6.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	78
2	Heptyl isobutyl carbonate		216	C12H24O3	959068-08-7	64
3	Heptane, 1,1'-oxybis-		214	C14H30O	000629-64-1	64
4	2-Propyl-1-pentanol		130	C8H18O	058175-57-8	45
5	2-Decene, 5-methyl-, (Z)-		154	C11H22	074645-86-6	45



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
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Acq On : 22 Jul 2017 7:24
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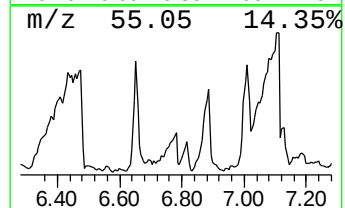
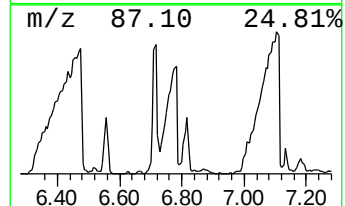
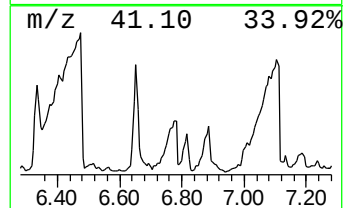
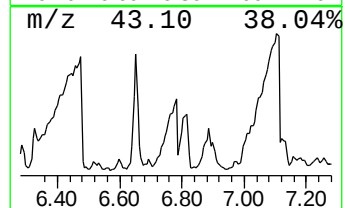
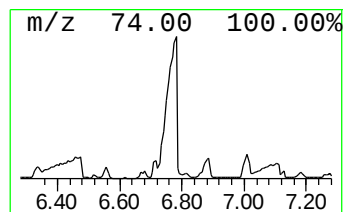
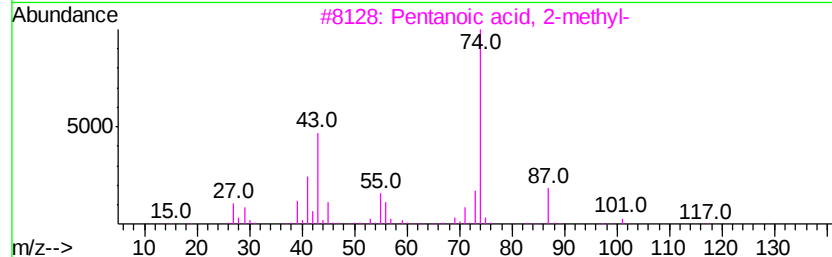
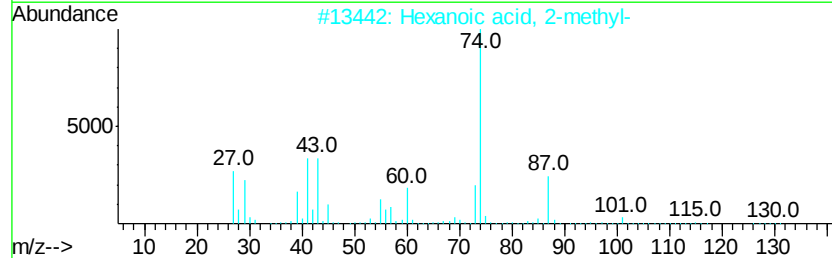
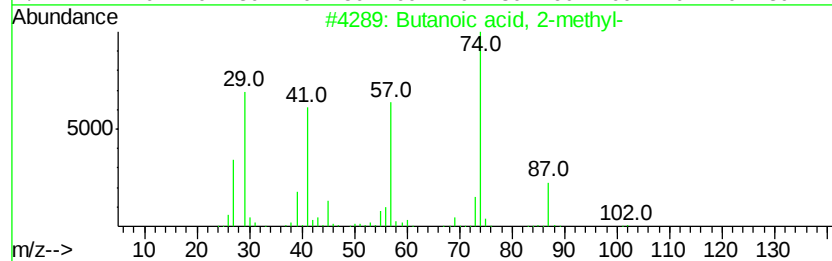
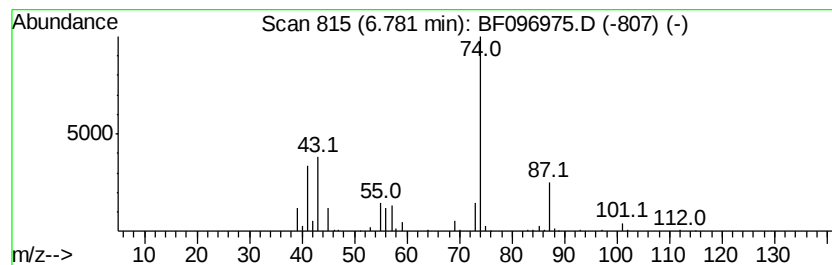
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Butanoic acid, 2-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	12.58 ng	492991	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	80
2		Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
3		Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	64
4		2-Methylheptanoic acid	144	C8H16O2	001188-02-9	50
5		1-Octadecanamine	269	C18H39N	000124-30-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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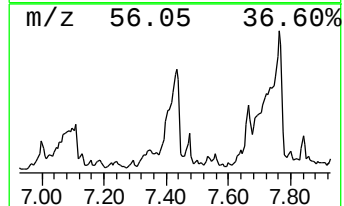
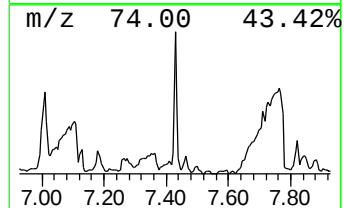
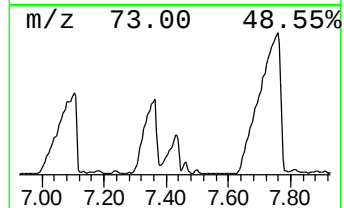
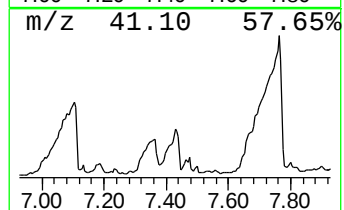
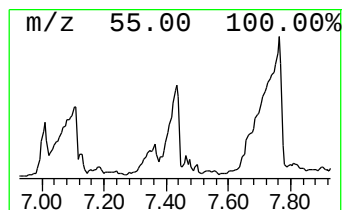
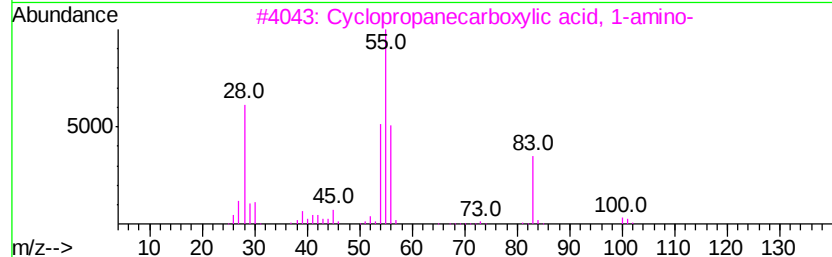
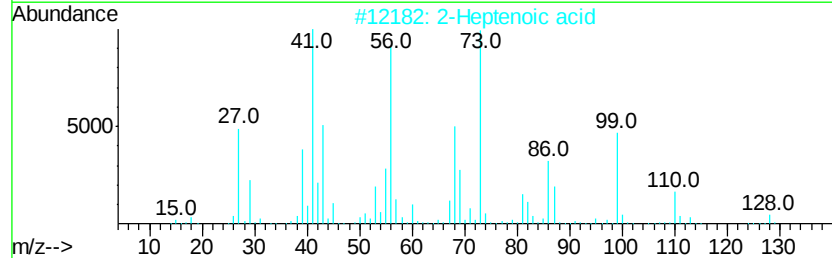
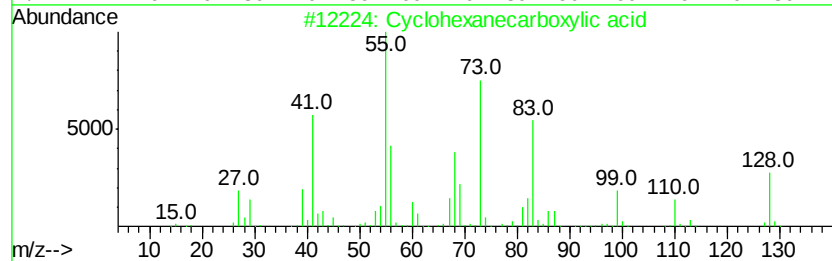
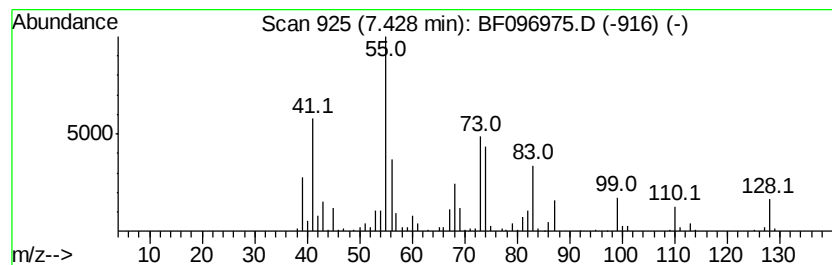
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexanecarboxylic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	21.39 ng	896346	Naphthalene-d8	7.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid	128	C7H12O2	000098-89-5	83
2			2-Heptenoic acid	128	C7H12O2	018999-28-5	35
3			Cyclopropanecarboxylic acid, 1-amino-	101	C4H7NO2	022059-21-8	25
4			Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	22
5			Trans-2-heptenoic acid	128	C7H12O2	1000342-31-8	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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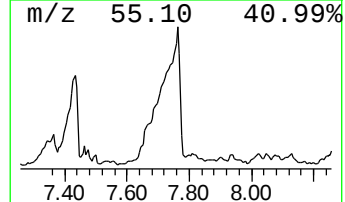
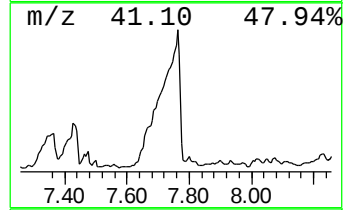
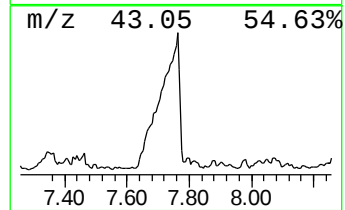
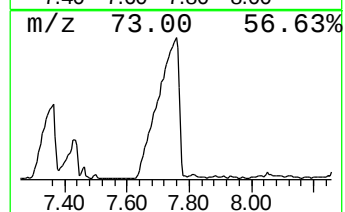
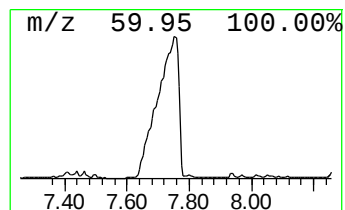
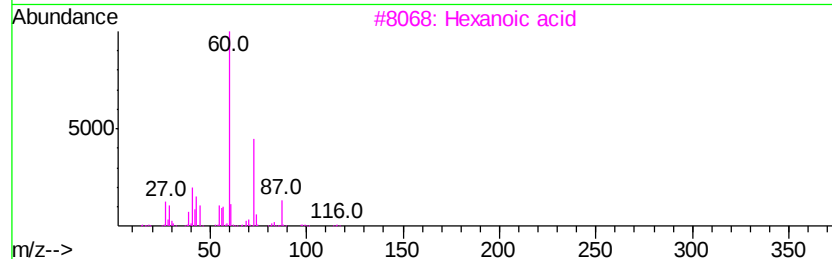
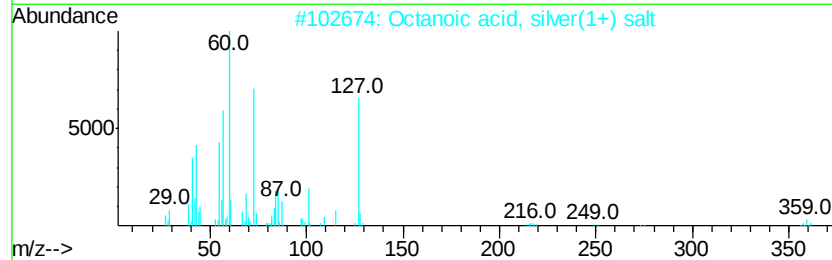
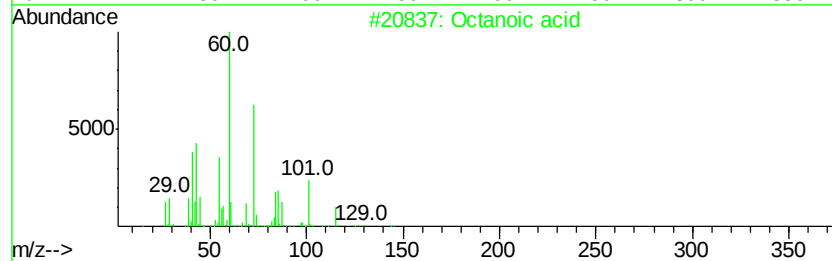
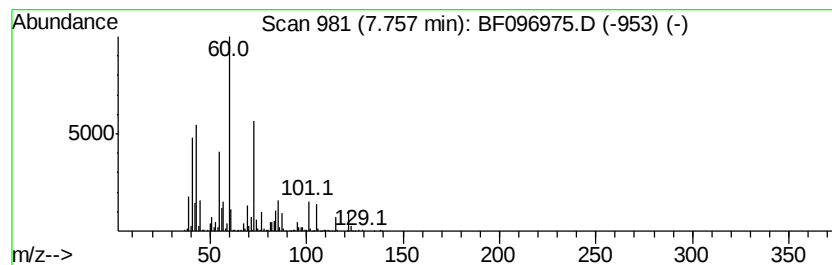
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.76	153.29 ng	6424380	Naphthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanoic acid	144	C8H16O2	000124-07-2	94
2		Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	59
3		Hexanoic acid	116	C6H12O2	000142-62-1	50
4		D-Fucose	164	C6H12O5	003615-37-0	43
5		Heptanoic acid	130	C7H14O2	000111-14-8	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096975.D
Acq On : 22 Jul 2017 7:24
Operator : SJ/JU
Sample : I4313-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

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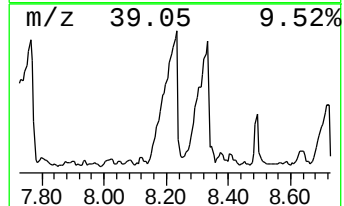
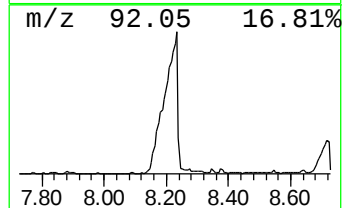
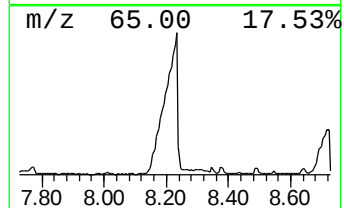
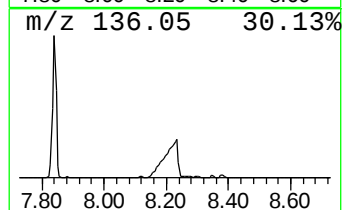
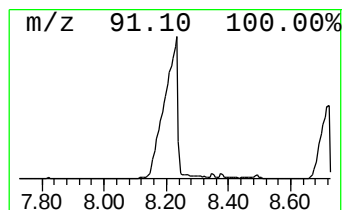
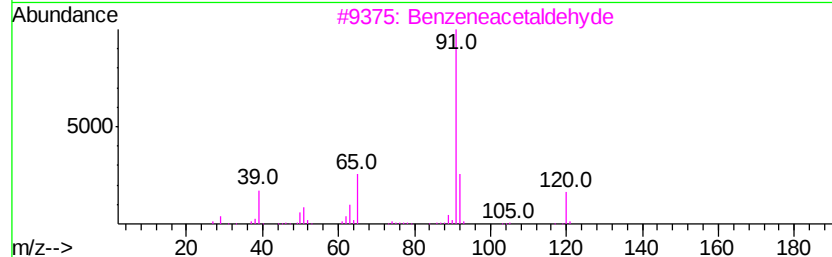
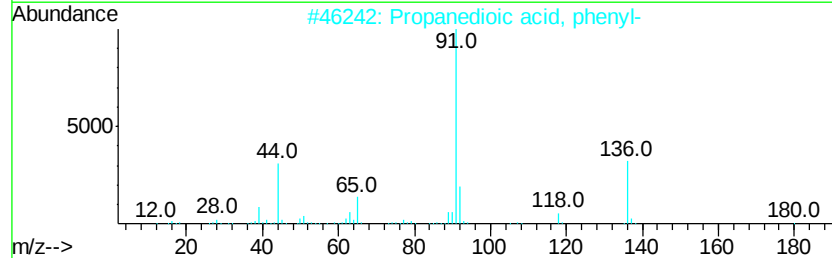
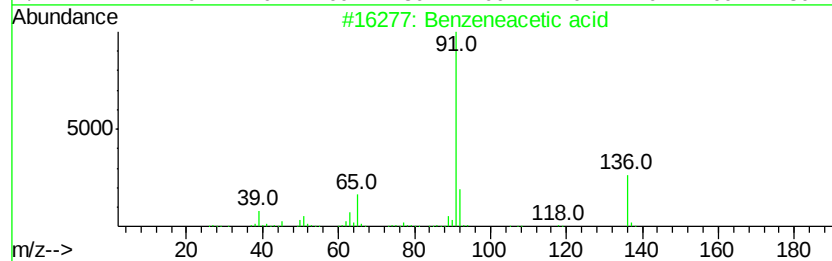
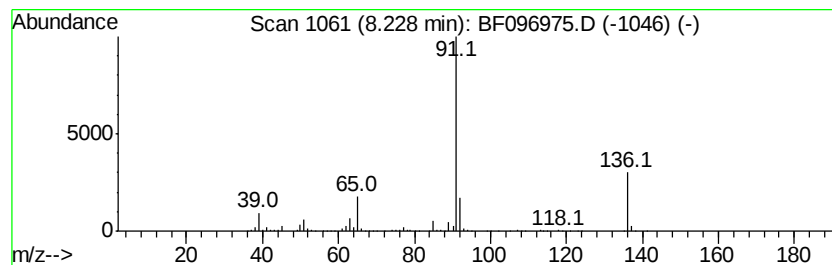
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Benzeneacetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.23	75.47 ng	3163070	Napthalene-d8	7.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	78
3			Benzeneacetaldehyde	120	C8H8O	000122-78-1	50
4			p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	50
5			3-Benzylsulfanyl-3-fluoro-2-trif...	294	C12H10F4O2S	1000275-92-0	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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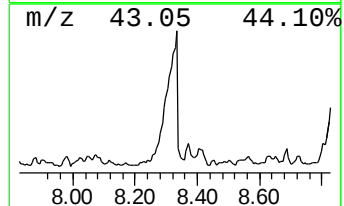
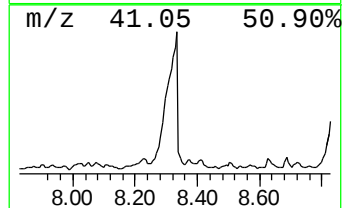
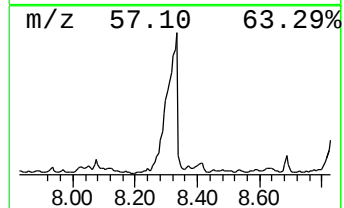
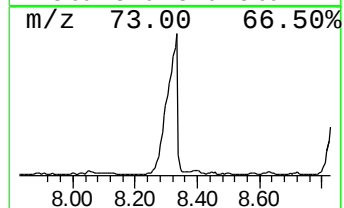
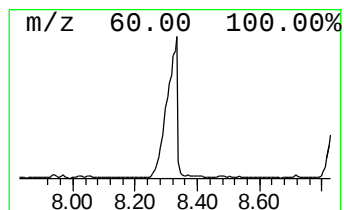
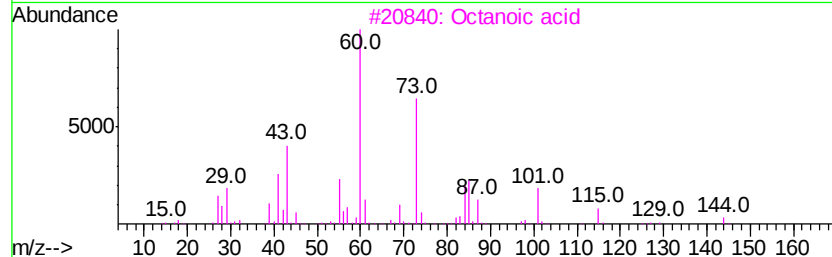
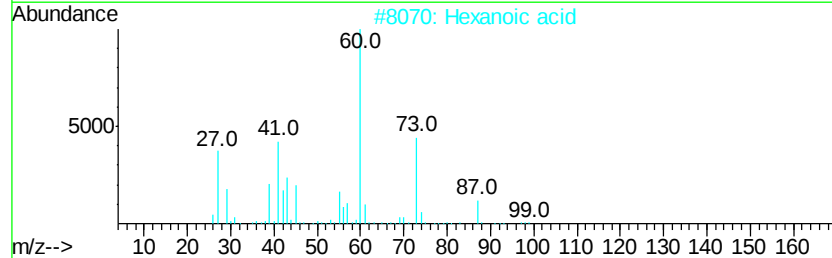
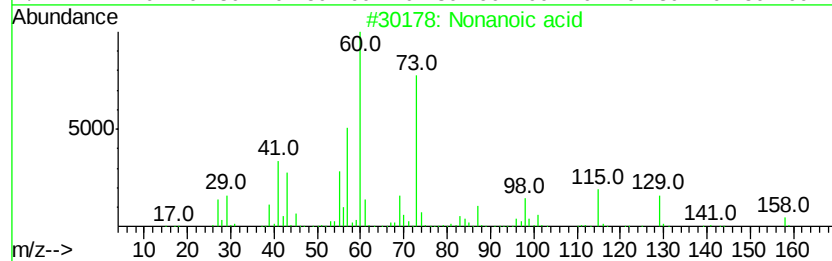
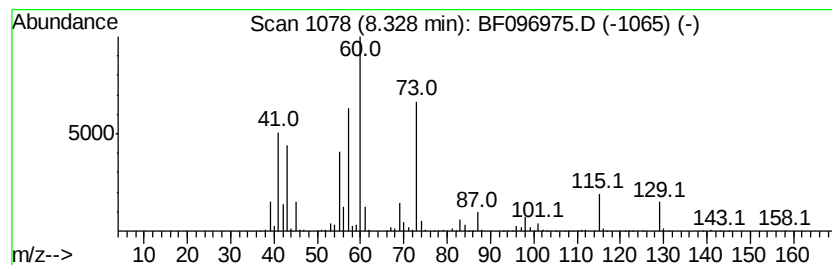
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Nonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.33	89.93 ng	3768870	Napthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	78
2		Hexanoic acid	116	C6H12O2	000142-62-1	64
3		Octanoic acid	144	C8H16O2	000124-07-2	64
4		Heptanoic acid	130	C7H14O2	000111-14-8	59
5		Pentanoic acid	102	C5H10O2	000109-52-4	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096975.D
Acq On : 22 Jul 2017 7:24
Operator : SJ/JU
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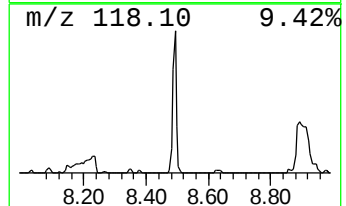
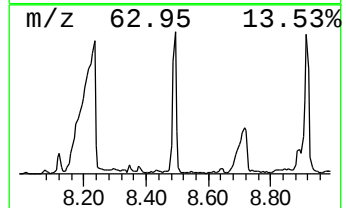
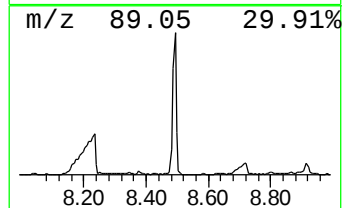
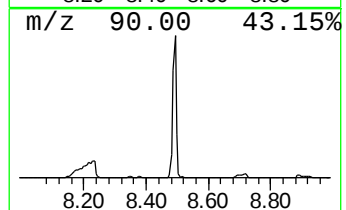
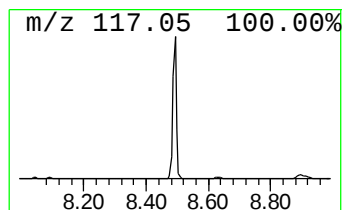
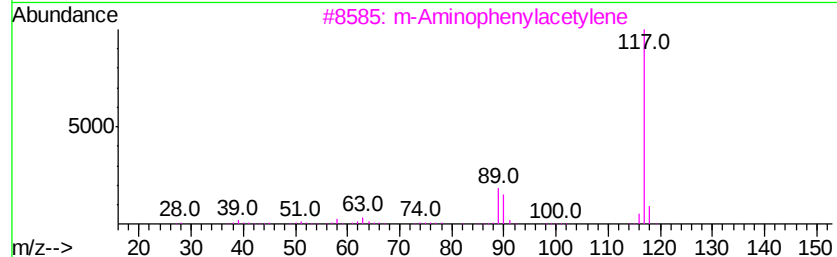
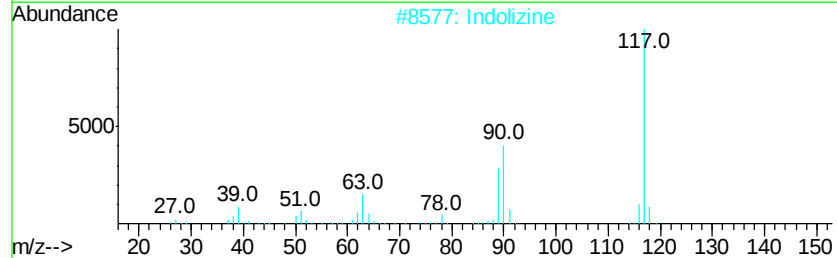
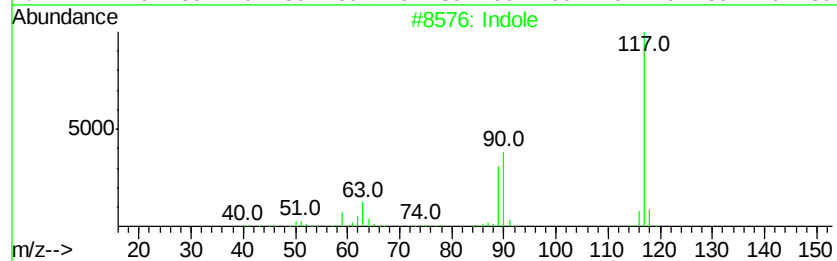
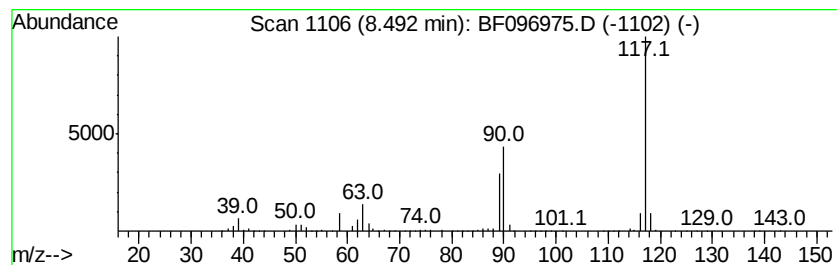
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Indole Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.49	15.38 ng	644675	Naphthalene-d8	7.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indole	117	C8H7N	000120-72-9	97
2		Indolizine	117	C8H7N	000274-40-8	90
3		m-Aminophenylacetylene	117	C8H7N	054060-30-9	87
4		5H-1-Pyrindine	117	C8H7N	000270-91-7	87
5		Benzyl nitrile	117	C8H7N	000140-29-4	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096975.D
Acq On : 22 Jul 2017 7:24
Operator : SJ/JU
Sample : I4313-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

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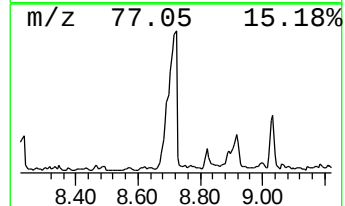
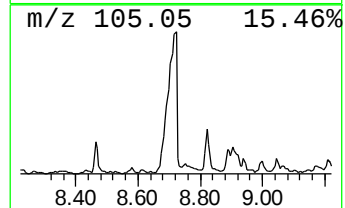
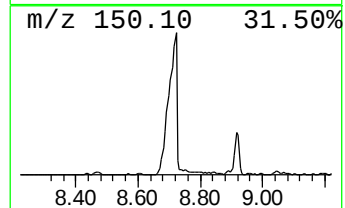
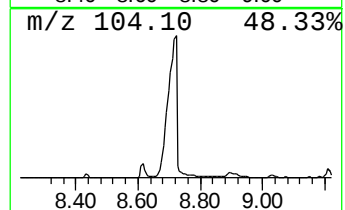
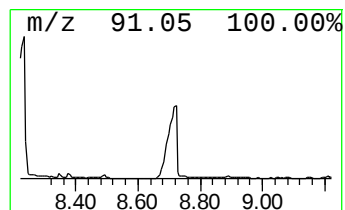
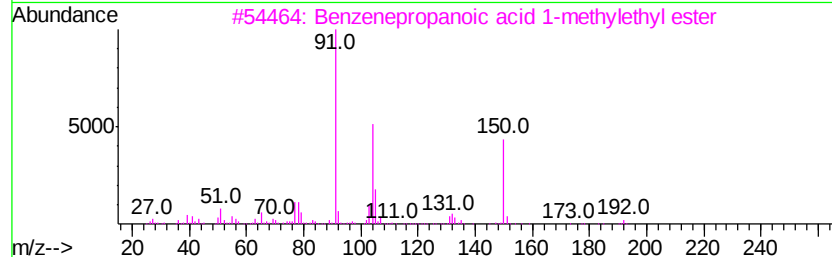
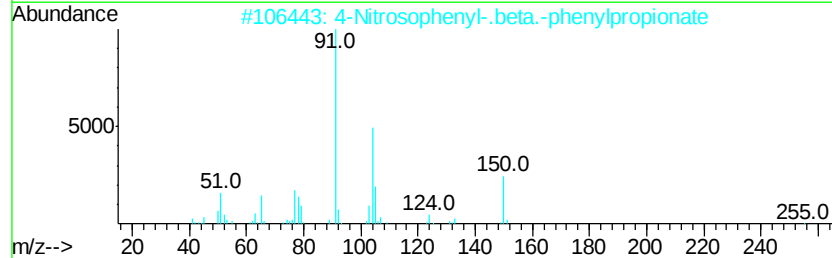
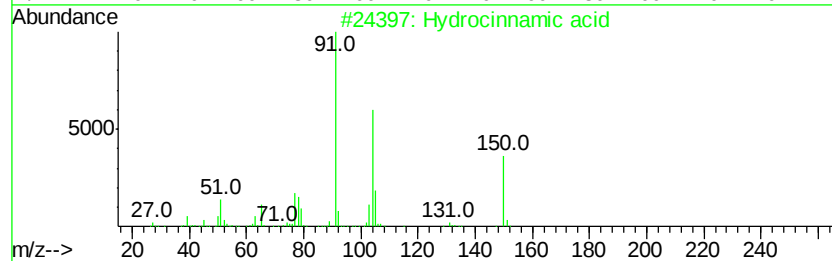
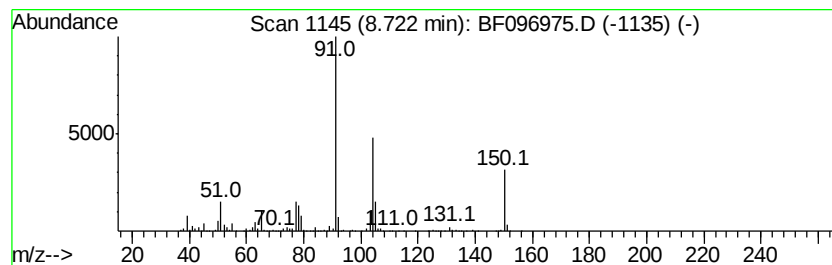
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Hydrocinnamic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	33.56 ng	1650970	Acenaphthene-d10	9.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrocinnamic acid	150	C9H10O2	000501-52-0	96
2		4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	86
3		Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	72
4		Benzenepropanoic acid, silver(1+...	256	C9H9AgO2	075112-79-7	72
5		Benzeneacetic acid, methyl ester	150	C9H10O2	000101-41-7	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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Acq On : 22 Jul 2017 7:24
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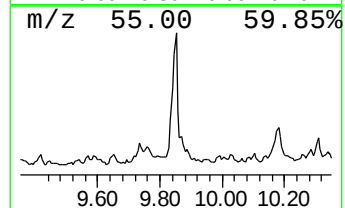
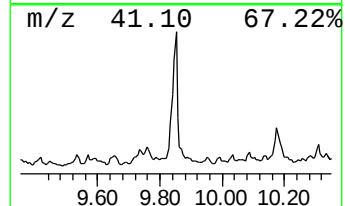
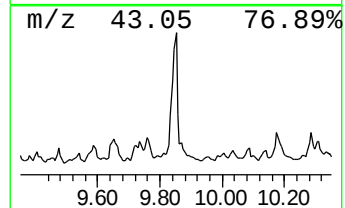
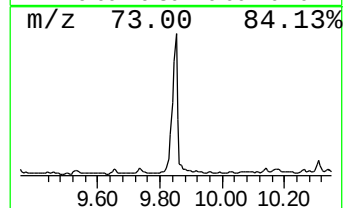
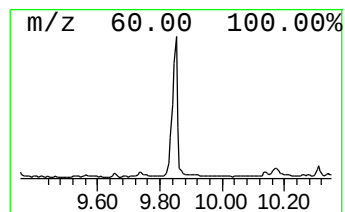
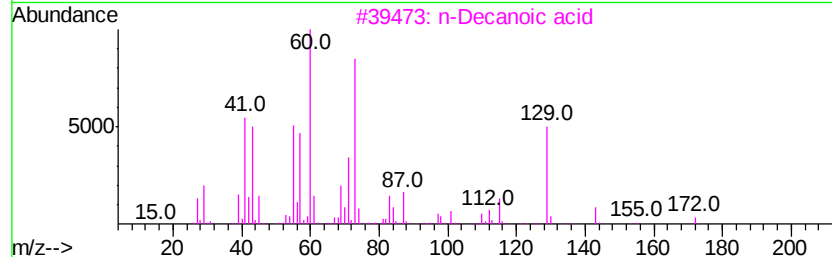
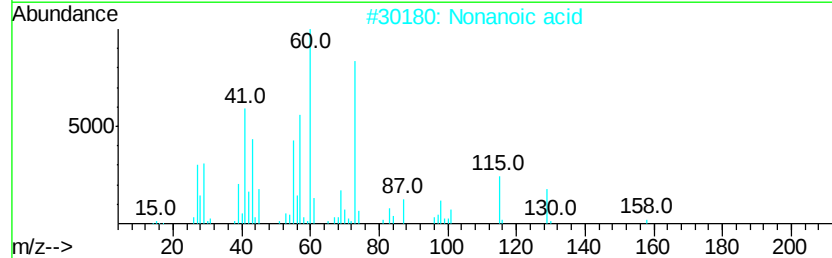
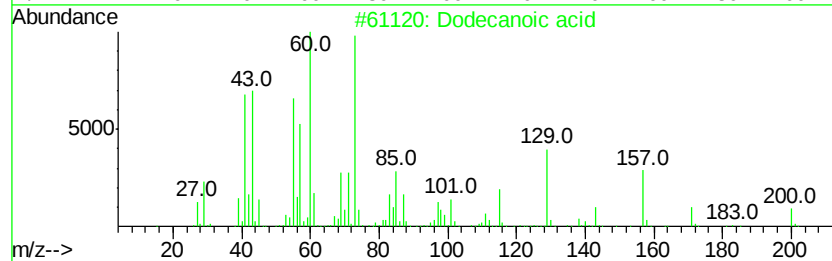
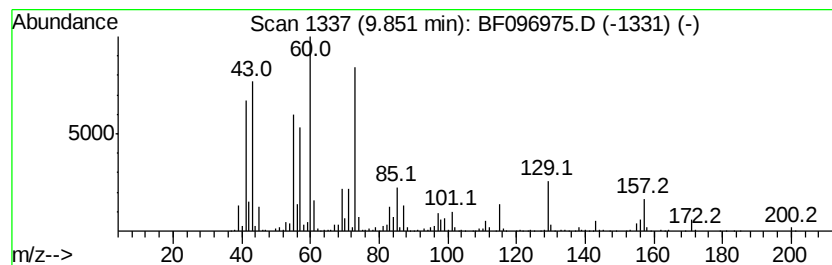
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Dodecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	28.08 ng	1381500	Acenaphthene-d10	9.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanoic acid	200	C12H24O2	000143-07-7	91
2		Nonanoic acid	158	C9H18O2	000112-05-0	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	53
4		Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43
5		Butanoic acid	88	C4H8O2	000107-92-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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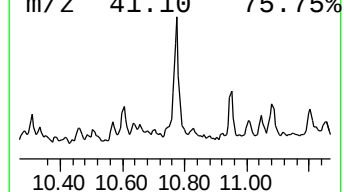
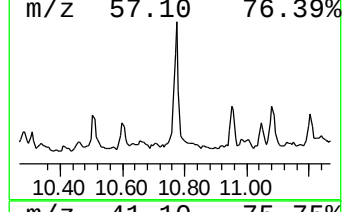
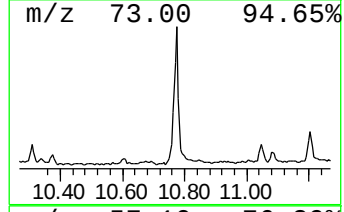
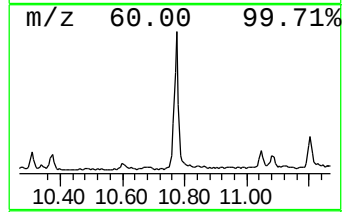
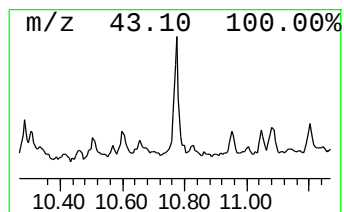
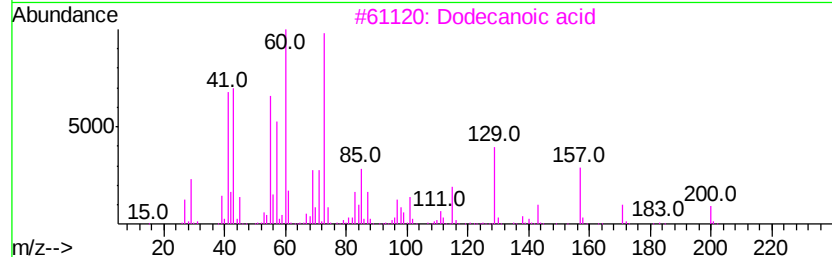
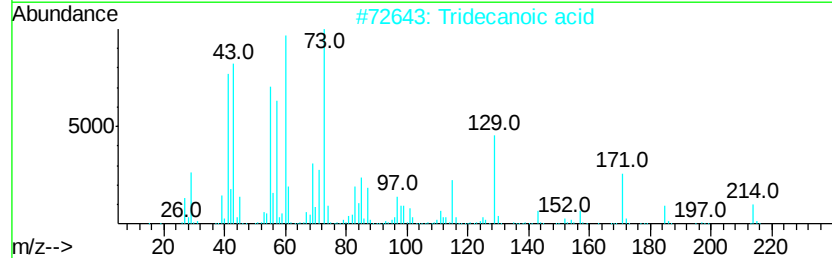
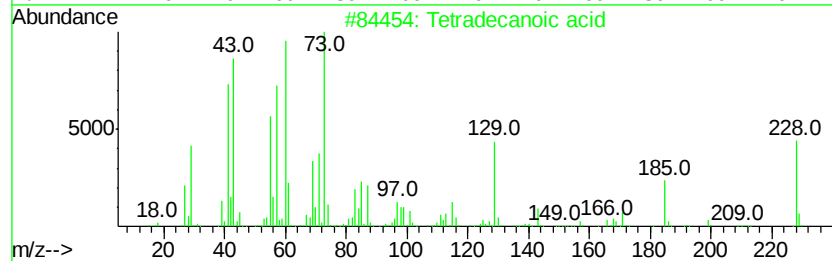
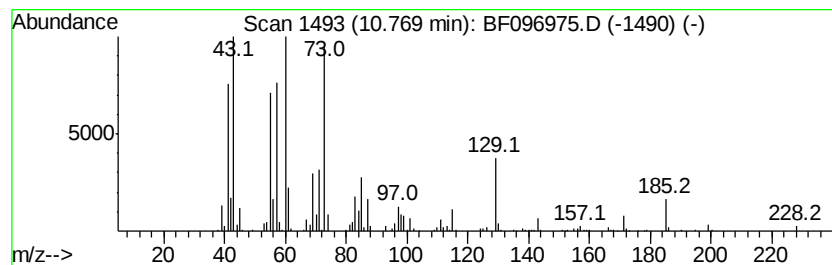
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Tetradecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.77	21.29 ng	845955	Phenanthrene-d10		11.06	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
2		Tridecanoic acid	214	C13H26O2	000638-53-9	87
3		Dodecanoic acid	200	C12H24O2	000143-07-7	86
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
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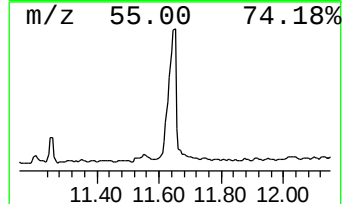
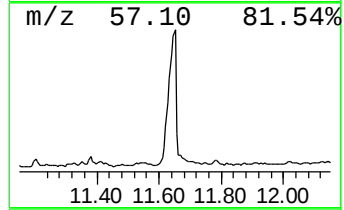
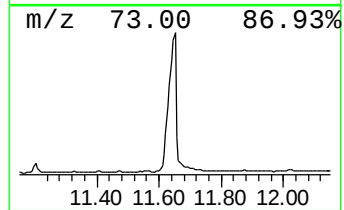
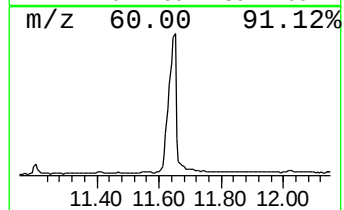
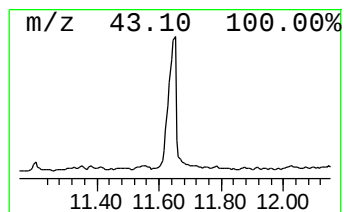
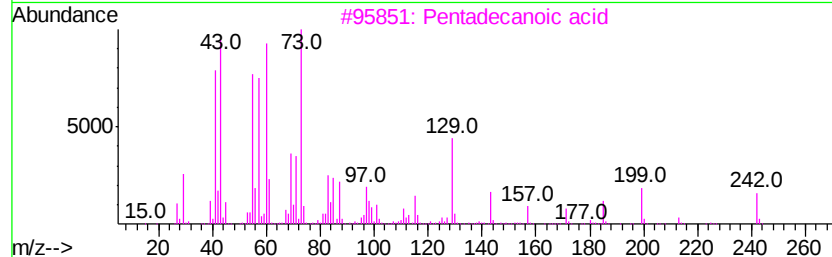
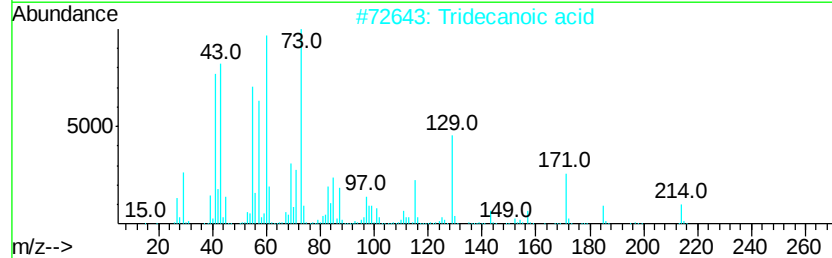
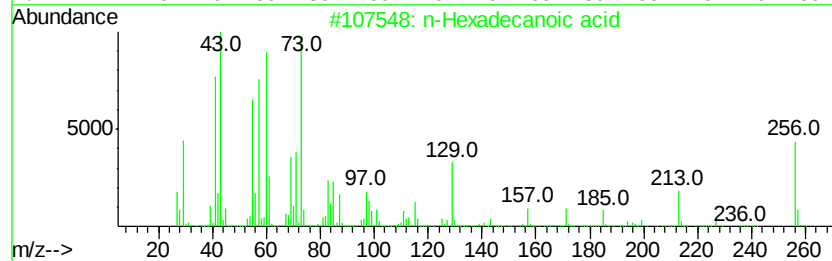
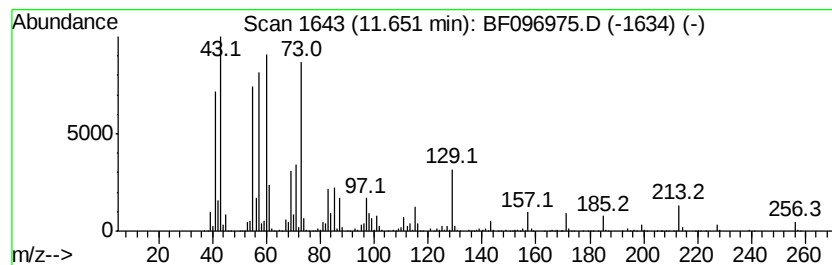
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BNA_F
ClientSampleId :
B-COMB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.65	129.52 ng	5146850	Phenanthrene-d10		11.06
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096975.D
Acq On : 22 Jul 2017 7:24
Operator : SJ/JU
Sample : I4313-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-COMB-1

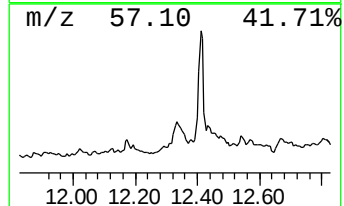
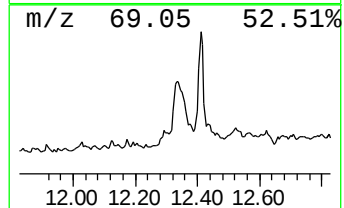
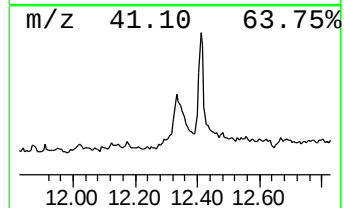
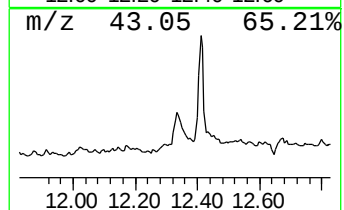
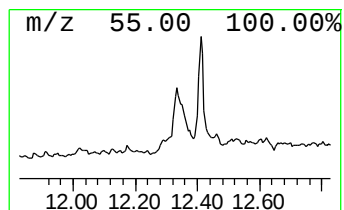
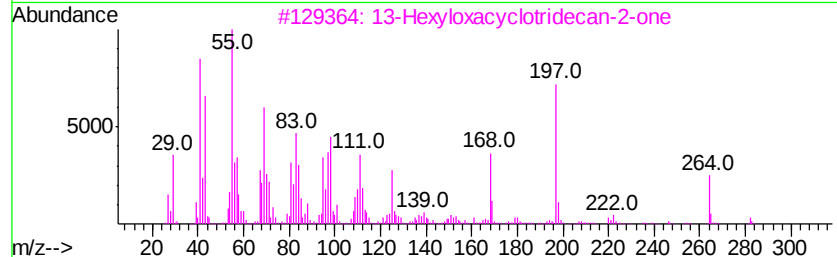
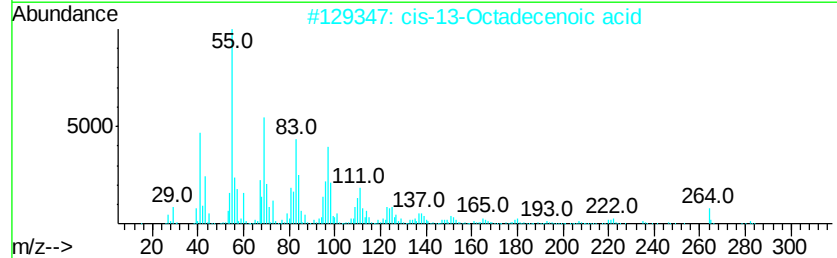
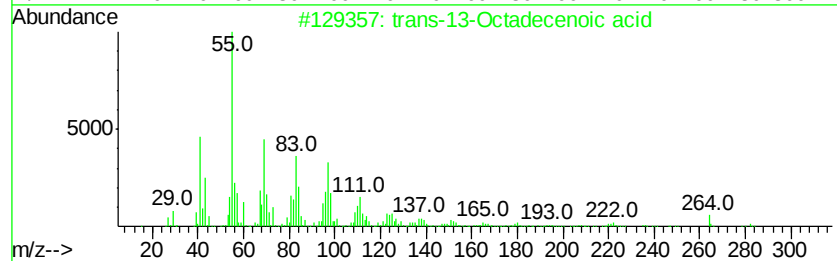
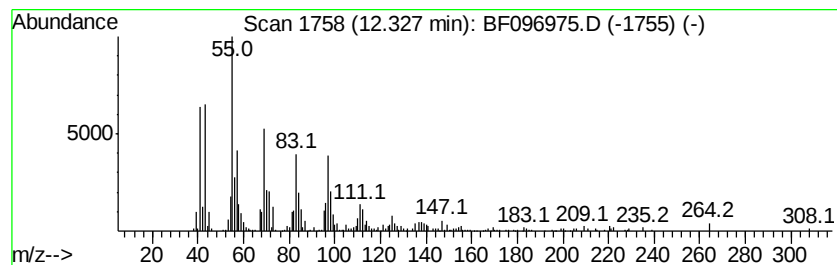
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 trans-13-Octadecenoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	18.29 ng	726689	Phenanthrene-d10	11.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	91
2		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	89
3		13-Hexyloxacyclotridecan-2-one	282	C18H34O2	000673-02-9	76
4		9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	74
5		cis-Vaccenic acid	282	C18H34O2	000506-17-2	68



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096975.D
Acq On : 22 Jul 2017 7:24
Operator : SJ/JU
Sample : I4313-03
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-COMB-1

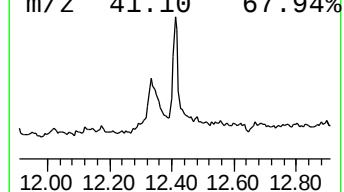
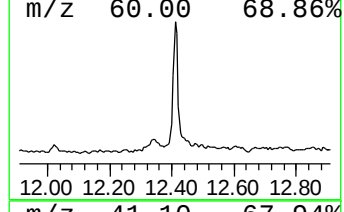
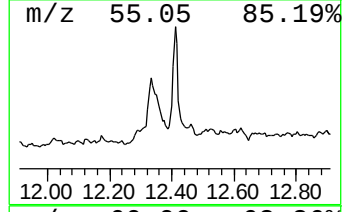
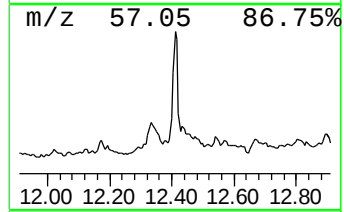
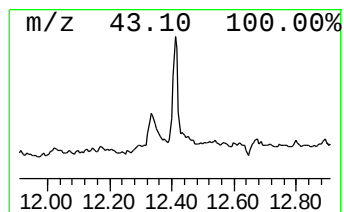
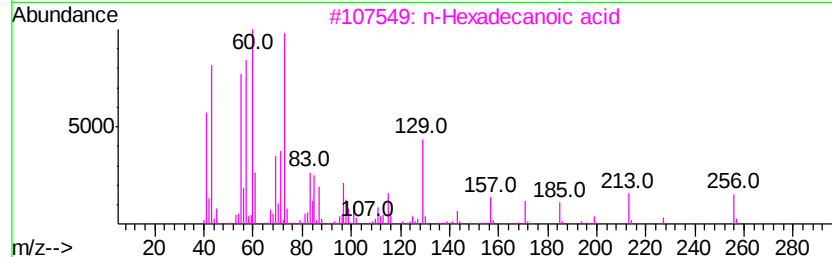
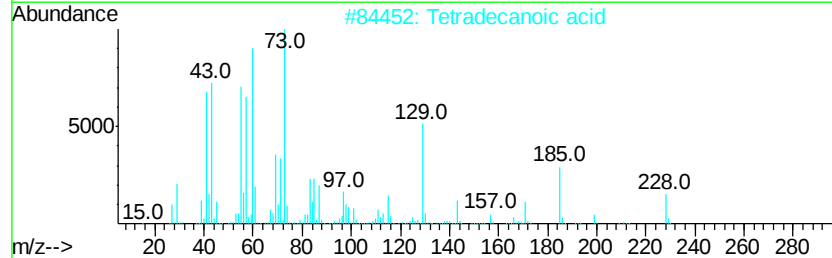
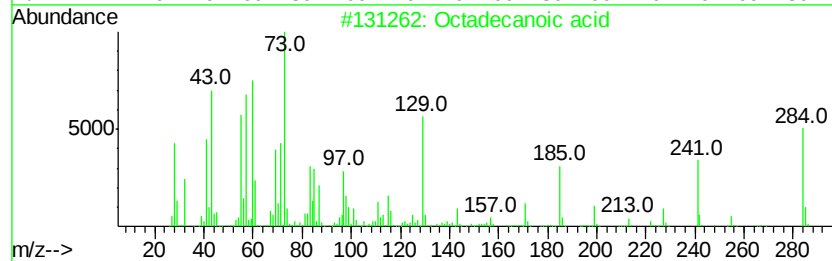
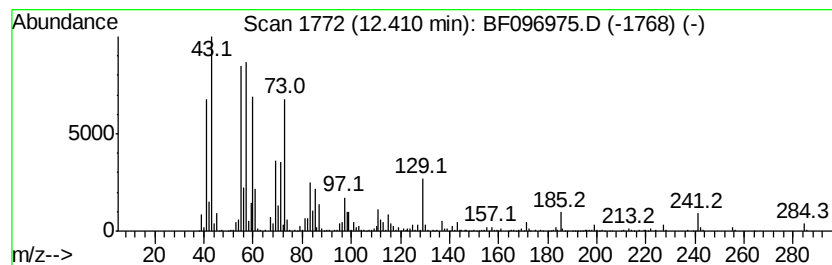
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	32.77 ng	1104490	Chrysene-d12	13.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	49
5		n-Decanoic acid	172	C10H20O2	000334-48-5	46



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
 Data File : BF096975.D
 Acq On : 22 Jul 2017 7:24
 Operator : SJ/JU
 Sample : I4313-03
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-COMB-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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
Butanoic acid, 3-...	5.06	21.9	ng	856448	1	6.56	784075	20.0
Butanoic acid	5.60	12.3	ng	482117	1	6.56	784075	20.0
Pentanoic acid	5.76	14.5	ng	566904	1	6.56	784075	20.0
Pentanoic acid, 2...	6.05	12.7	ng	499182	1	6.56	784075	20.0
unknown6.33	6.33	50.7	ng	1987590	1	6.56	784075	20.0
Hexanoic acid	6.41	13.1	ng	514901	1	6.56	784075	20.0
1-Hexanol, 2-ethyl-	6.65	13.4	ng	527127	1	6.56	784075	20.0
Butanoic acid, 2-...	6.78	12.6	ng	492991	1	6.56	784075	20.0
Cyclohexanecarbox...	7.43	21.4	ng	896346	2	7.84	838184	20.0
Octanoic acid	7.76	153.3	ng	6424380	2	7.84	838184	20.0
Benzeneacetic acid	8.23	75.5	ng	3163070	2	7.84	838184	20.0
Nonanoic acid	8.33	89.9	ng	3768870	2	7.84	838184	20.0
Indole	8.49	15.4	ng	644675	2	7.84	838184	20.0
Hydrocinnamic acid	8.72	33.6	ng	1650970	3	9.59	983904	20.0
Dodecanoic acid	9.85	28.1	ng	1381500	3	9.59	983904	20.0
Tetradecanoic acid	10.77	21.3	ng	845955	4	11.06	794758	20.0
n-Hexadecanoic acid	11.65	129.5	ng	5146850	4	11.06	794758	20.0
trans-13-Octadece...	12.33	18.3	ng	726689	4	11.06	794758	20.0
Octadecanoic acid	12.41	32.8	ng	1104490	5	13.69	674093	20.0