

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
 Data File : BF086734.D
 Acq On : 6 May 2016 20:04
 Operator : UM/SJ
 Sample : H2802-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

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-BF050416.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	3.516	122	125	131	rBV	74328	151190	2.34%	0.271%
2	4.041	169	171	175	rBV	59662	97268	1.50%	0.174%
3	4.796	233	237	244	rBV5	32297	128043	1.98%	0.230%
4	4.910	244	247	250	rVV	84607	171612	2.65%	0.308%
5	5.013	254	256	261	rVB	54027	79626	1.23%	0.143%
6	5.242	274	276	280	rBV	89331	177046	2.74%	0.318%
7	5.310	280	282	285	rBV	1817829	2318032	35.83%	4.157%
8	5.493	296	298	303	rVB2	196775	272206	4.21%	0.488%
9	5.573	303	305	312	rVB	73230	110428	1.71%	0.198%
10	5.676	312	314	316	rBV	116828	141420	2.19%	0.254%
11	5.722	316	318	319	rVV	88969	95563	1.48%	0.171%
12	5.744	319	320	326	rVB	45948	89222	1.38%	0.160%
13	5.893	331	333	338	rBV	187661	277568	4.29%	0.498%
14	5.962	338	339	344	rBV3	53533	89279	1.38%	0.160%
15	6.144	354	355	360	rVB	327762	495735	7.66%	0.889%
16	6.224	360	362	366	rBV3	78805	133708	2.07%	0.240%
17	6.304	366	369	372	rBV3	147521	294889	4.56%	0.529%
18	6.373	372	375	379	rVV	1502028	1755486	27.14%	3.148%
19	6.442	379	381	382	rVV	423059	499034	7.71%	0.895%
20	6.487	382	385	387	rVV	4143879	5118710	79.12%	9.180%
21	6.533	387	389	390	rVV	78327	98181	1.52%	0.176%
22	6.556	390	391	394	rVB2	73740	104059	1.61%	0.187%
23	6.602	394	395	399	rVB2	49938	67573	1.04%	0.121%
24	6.705	402	404	407	rBV	1242127	1197837	18.52%	2.148%
25	6.762	407	409	414	rBV2	220840	335246	5.18%	0.601%
26	6.865	415	418	420	rVV	4342665	4759605	73.57%	8.536%
27	6.956	422	426	429	rBV	189010	310276	4.80%	0.556%
28	7.013	429	431	432	rVV	159516	141788	2.19%	0.254%
29	7.059	432	435	438	rVB2	200364	283728	4.39%	0.509%
30	7.139	438	442	445	rBV	330099	687512	10.63%	1.233%
31	7.207	445	448	451	rVB4	114059	206074	3.19%	0.370%
32	7.287	451	455	457	rBV	2624784	4562301	70.52%	8.182%
33	7.413	464	466	469	rVB2	149428	204743	3.16%	0.367%
34	7.482	469	472	475	rVB4	42709	95218	1.47%	0.171%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
 Data File : BF086734.D
 Acq On : 6 May 2016 20:04
 Operator : UM/SJ
 Sample : H2802-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

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-BF050416.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	7.550	476	478	481	rVB3	80226	125113	1.93%	0.224%
36	7.607	481	483	486	rBV3	39723	90122	1.39%	0.162%
37	7.665	486	488	491	rVB2	135895	174833	2.70%	0.314%
38	7.722	491	493	495	rBV	221662	268603	4.15%	0.482%
39	7.790	495	499	503	rBV5	258316	597173	9.23%	1.071%
40	7.882	503	507	508	rBV4	61235	103191	1.60%	0.185%
41	7.927	508	511	514	rBV2	73701	125574	1.94%	0.225%
42	7.996	514	517	519	rVB	1436292	1544437	23.87%	2.770%
43	8.088	523	525	528	rVB2	68691	92013	1.42%	0.165%
44	8.133	528	529	531	rBV2	70265	104353	1.61%	0.187%
45	8.282	540	542	544	rBV	100025	138011	2.13%	0.248%
46	8.385	547	551	555	rBV2	355101	682039	10.54%	1.223%
47	8.453	555	557	559	rBV2	70272	88617	1.37%	0.159%
48	8.590	566	569	573	rVB4	112664	212127	3.28%	0.380%
49	8.659	573	575	576	rBV2	44322	70323	1.09%	0.126%
50	8.693	576	578	581	rVB2	101503	173084	2.68%	0.310%
51	8.739	581	582	584	rBV2	66626	102635	1.59%	0.184%
52	8.785	584	586	587	rVV2	93147	113436	1.75%	0.203%
53	8.888	591	595	597	rBV4	77684	191935	2.97%	0.344%
54	8.945	598	600	602	rVV2	136903	230886	3.57%	0.414%
55	9.002	602	605	607	rVV2	286231	495687	7.66%	0.889%
56	9.070	607	611	614	rVV	4654028	6469249	100.00%	11.602%
57	9.173	617	620	623	rVB4	89801	183602	2.84%	0.329%
58	9.230	623	625	631	rVB3	188369	333928	5.16%	0.599%
59	9.322	631	633	634	rBV2	92782	158546	2.45%	0.284%
60	9.436	641	643	645	rVB	83670	117965	1.82%	0.212%
61	9.470	645	646	649	rBV3	80593	115331	1.78%	0.207%
62	9.573	654	655	657	rVV	97827	102886	1.59%	0.185%
63	9.619	657	659	660	rVV	122956	119245	1.84%	0.214%
64	9.688	662	665	667	rVV3	122862	257976	3.99%	0.463%
65	9.745	667	670	672	rVV	1833493	1779635	27.51%	3.192%
66	9.825	676	677	681	rVB4	60580	92034	1.42%	0.165%
67	9.928	683	686	687	rBV2	50293	86077	1.33%	0.154%
68	10.053	695	697	701	rVB4	74682	138185	2.14%	0.248%
69	10.179	706	708	710	rVB	296851	313332	4.84%	0.562%
70	10.236	710	713	714	rBV3	43573	72807	1.13%	0.131%
71	10.533	736	739	742	rVB	3304309	3993456	61.73%	7.162%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

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:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	10.648	747	749	751	rBV	96921	110450	1.71%	0.198%
73	10.751	756	758	760	rBV2	85047	94658	1.46%	0.170%
74	10.911	770	772	776	rVV4	71594	113313	1.75%	0.203%
75	10.979	776	778	781	rVB	94513	128125	1.98%	0.230%
76	11.219	797	799	802	rBV	1495489	1449994	22.41%	2.601%
77	11.276	802	804	808	rVB2	51913	108990	1.68%	0.195%
78	11.768	844	847	851	rBV3	359359	409688	6.33%	0.735%
79	12.477	905	909	913	rBV5	32020	95310	1.47%	0.171%
80	12.545	913	915	921	rVB	323762	363930	5.63%	0.653%
81	12.808	935	938	940	rBV	4510192	4690166	72.50%	8.412%
82	12.842	940	941	944	rVB	288797	257155	3.98%	0.461%
83	13.699	1014	1016	1020	rBV	106843	151355	2.34%	0.271%
84	13.848	1027	1029	1032	rBV	1277427	1207125	18.66%	2.165%
85	15.231	1147	1150	1159	rVB	728355	968618	14.97%	1.737%

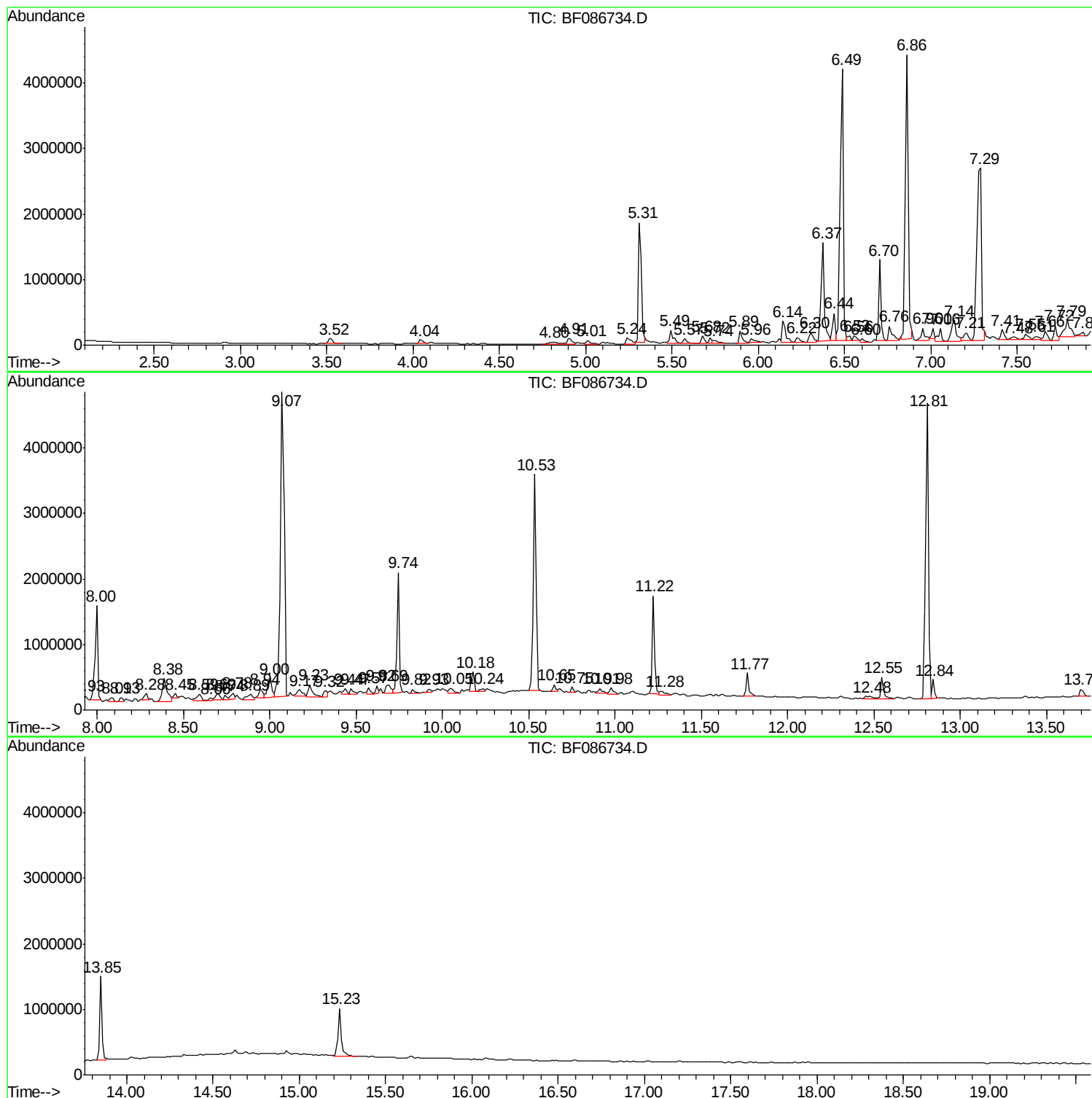
Sum of corrected areas: 55757529

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

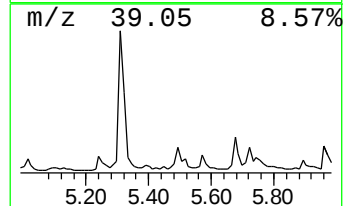
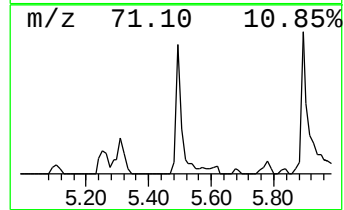
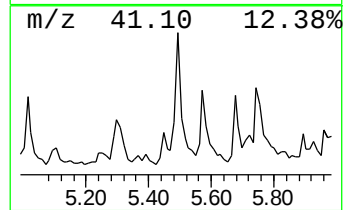
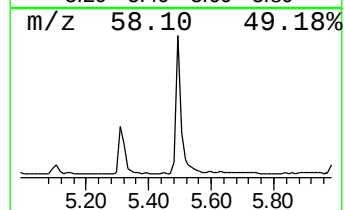
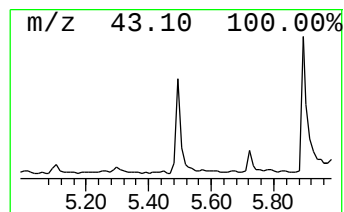
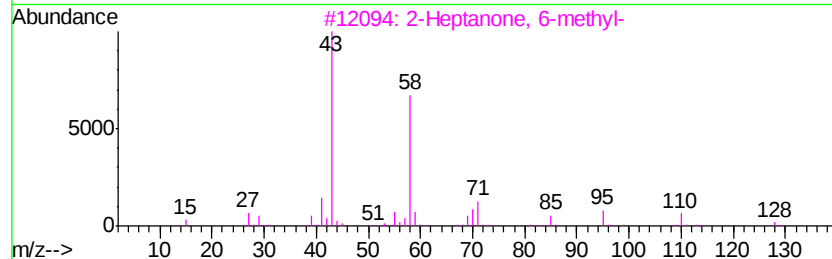
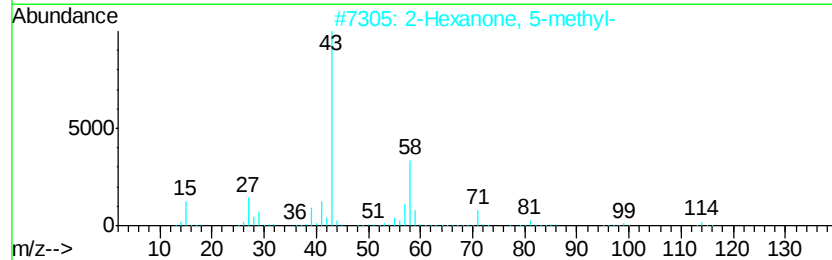
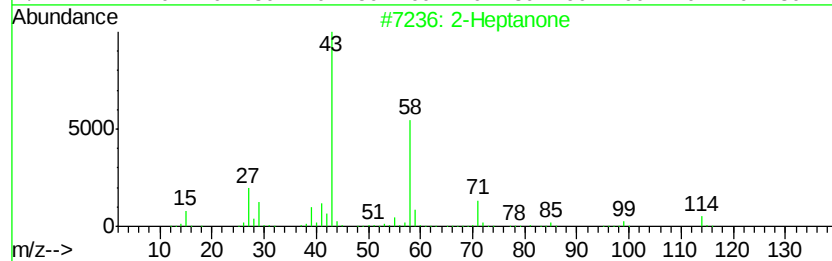
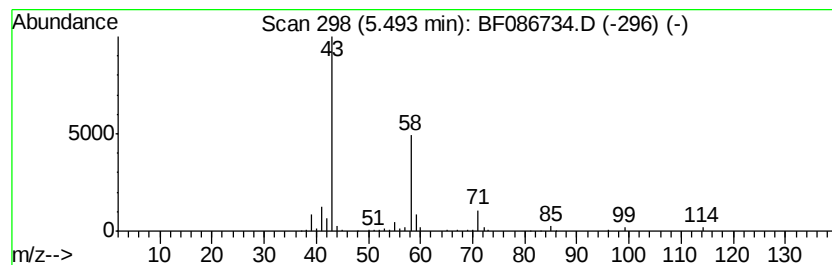
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Heptanone Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.49	9.09 ng	272206	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanone	114	C7H14O	000110-43-0	78
2		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	58
3		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	50
4		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	45
5		2-Hexanone	100	C6H12O	000591-78-6	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

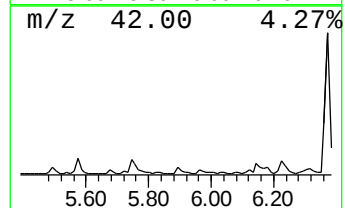
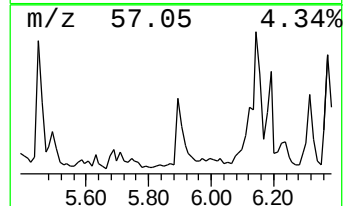
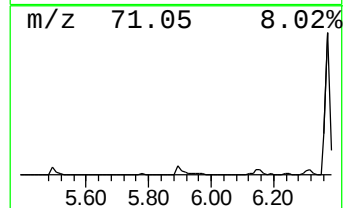
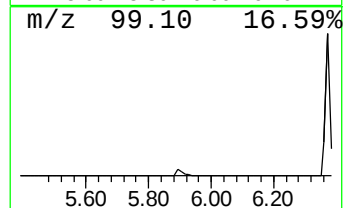
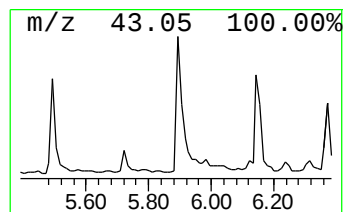
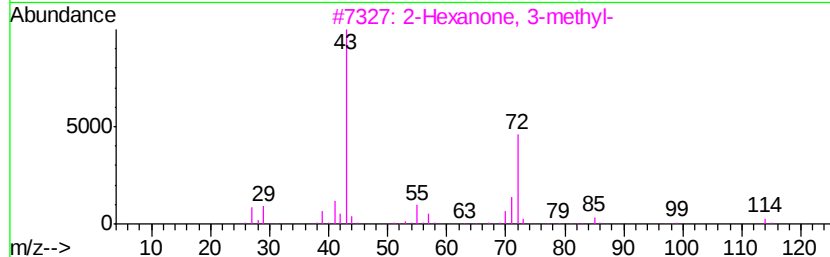
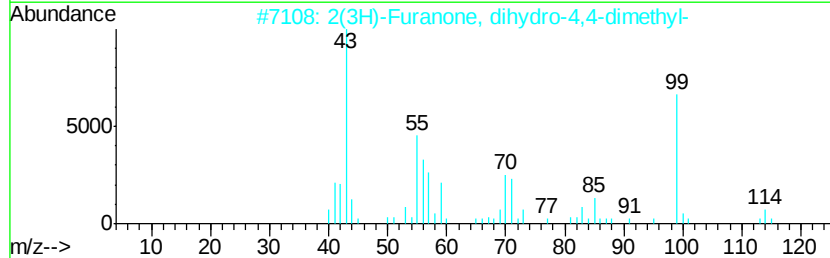
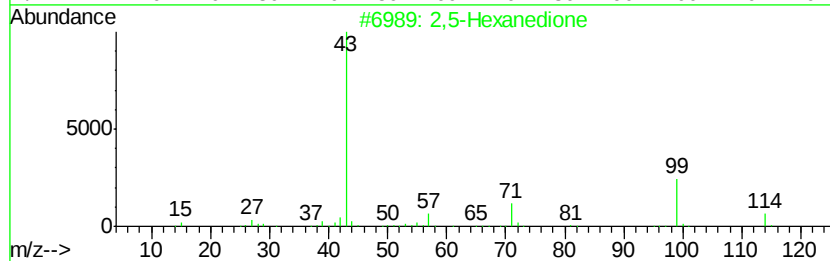
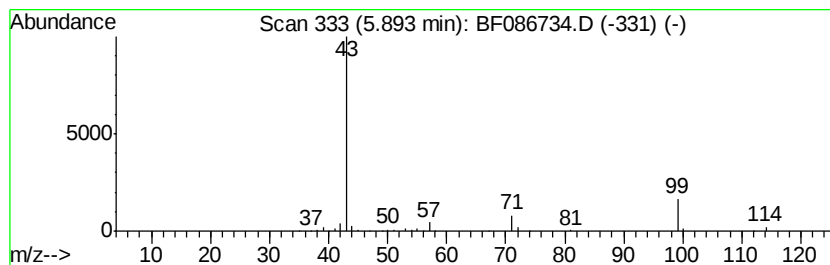
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2,5-Hexanedione Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	9.27 ng	277568	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Hexanedione	114	C6H10O2	000110-13-4	64
2	2(3H)-Furanone, dihydro-4,4-dime...	114	C6H10O2	013861-97-7	32
3	2-Hexanone, 3-methyl-	114	C7H14O	002550-21-2	32
4	Vinyl butyrate	114	C6H10O2	000123-20-6	9
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

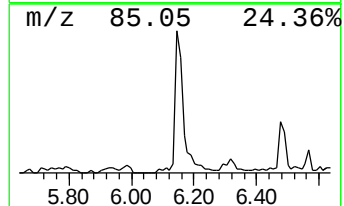
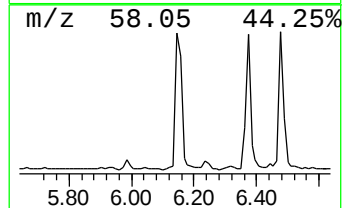
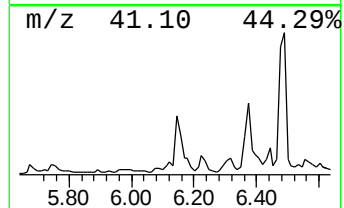
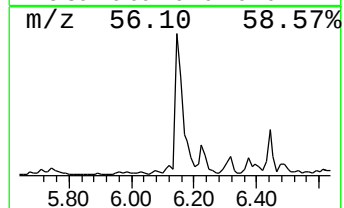
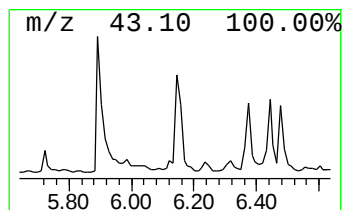
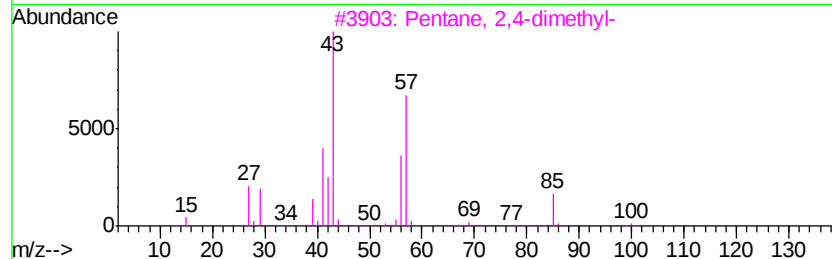
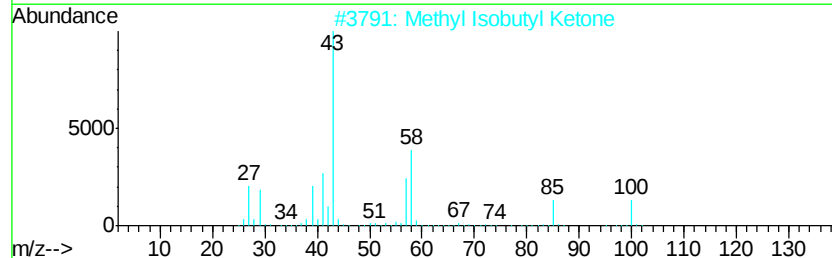
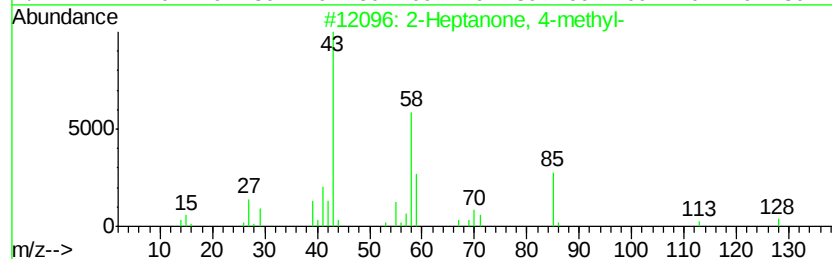
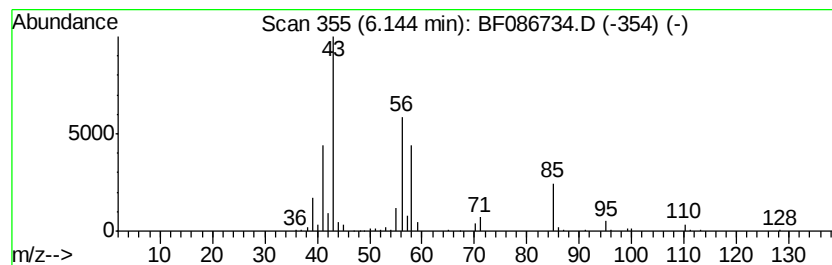
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.14 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.14	16.55 ng	495735	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	47
2		Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	38
3		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	35
4		Hexane, 1-propoxy-	144	C9H20O	053685-78-2	27
5		2(3H)-Furanone, dihydro-5-methyl-	100	C5H8O2	000108-29-2	25



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

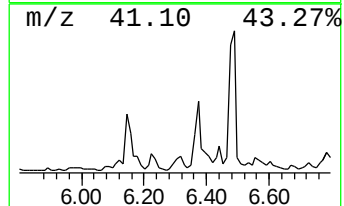
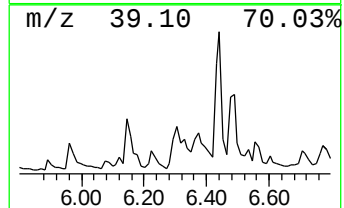
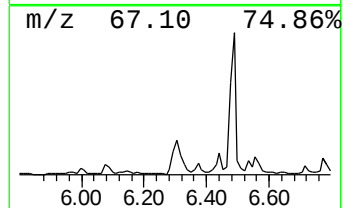
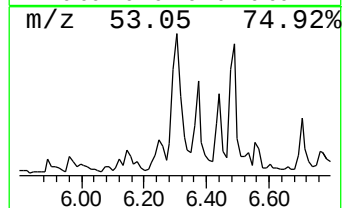
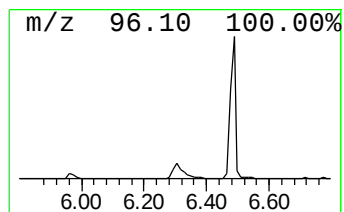
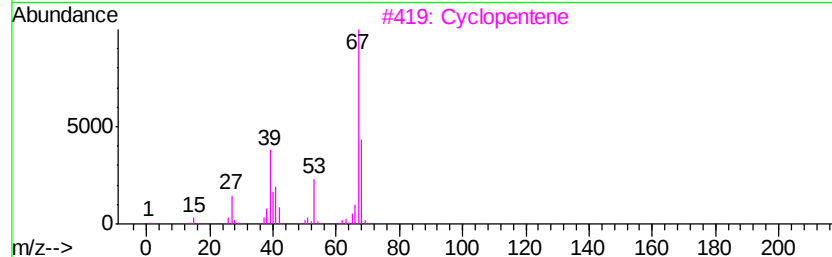
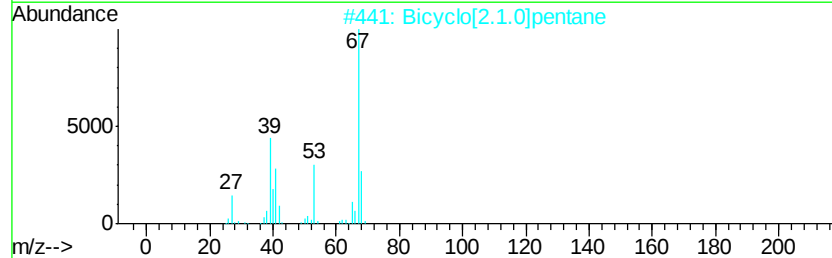
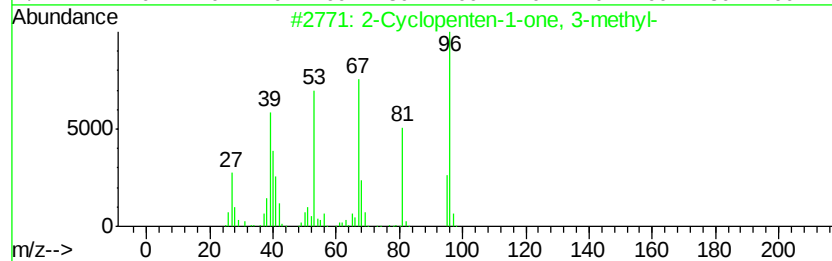
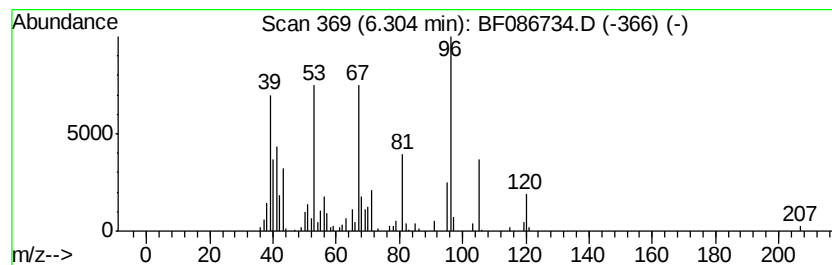
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Cyclopenten-1-one, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.30	9.85 ng	294889	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	95
2		Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	94
3		Cyclopentene	68	C5H8	000142-29-0	86
4		2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	001120-73-6	83
5		1,3-Butadiene, 2-methyl-	68	C5H8	000078-79-5	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

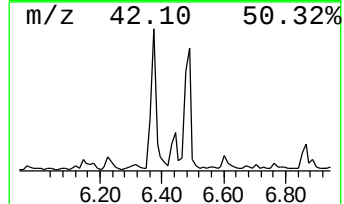
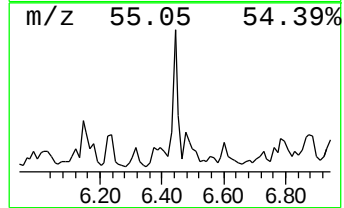
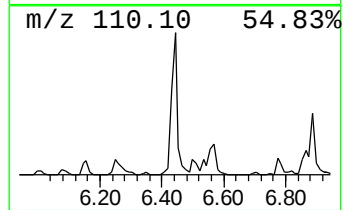
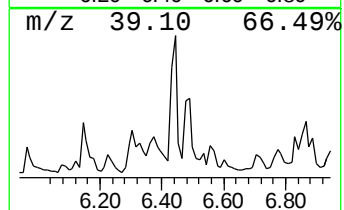
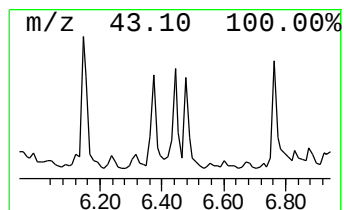
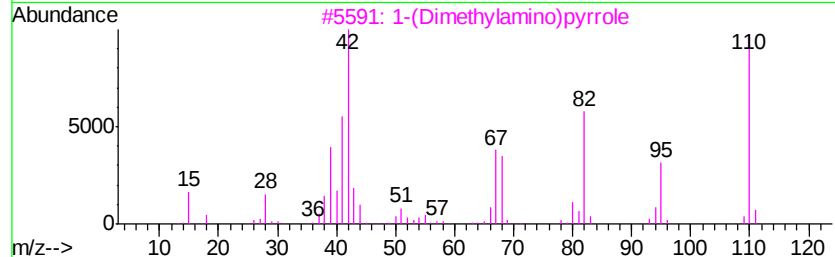
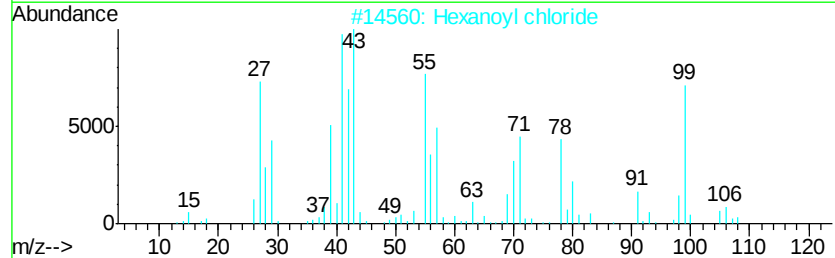
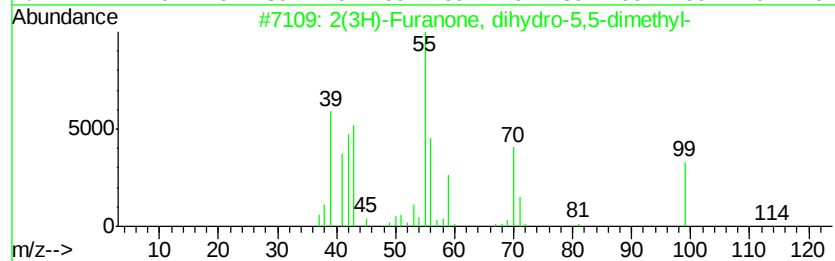
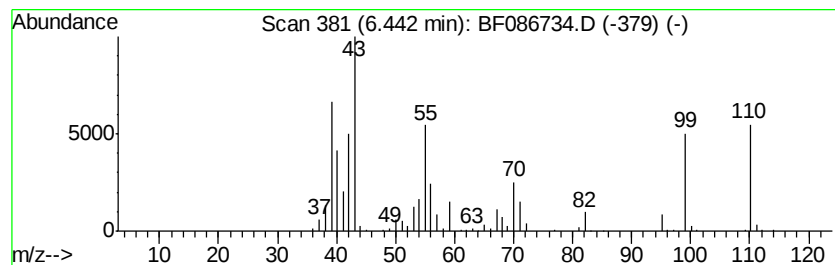
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2(3H)-Furanone, dihydro-5,5... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.44	16.66 ng	499034	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, dihydro-5,5-dime...	114	C6H10O2	003123-97-5	86
2		Hexanoyl chloride	134	C6H11ClO	000142-61-0	37
3		1-(Dimethylamino)pyrrole	110	C6H10N2	078307-76-3	35
4		1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	32
5		4(3H)-Pyrimidinone, 3-methyl-	110	C5H6N2O	006104-45-6	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

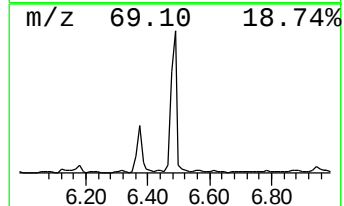
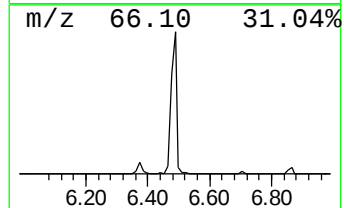
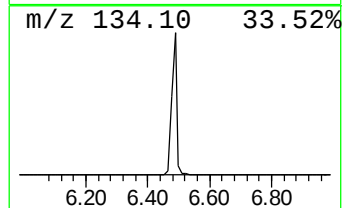
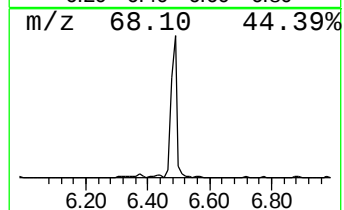
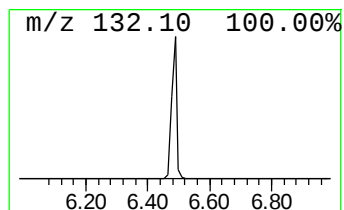
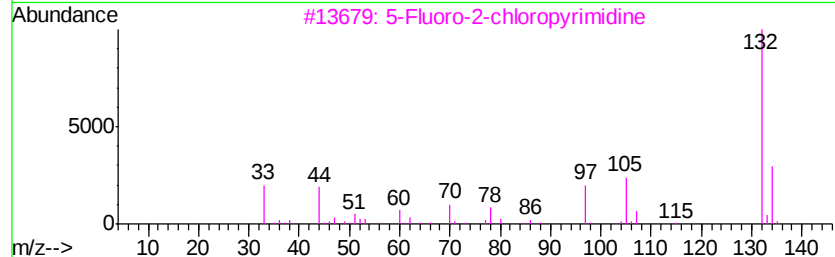
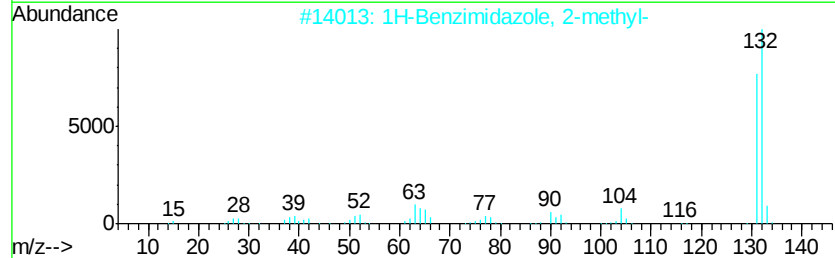
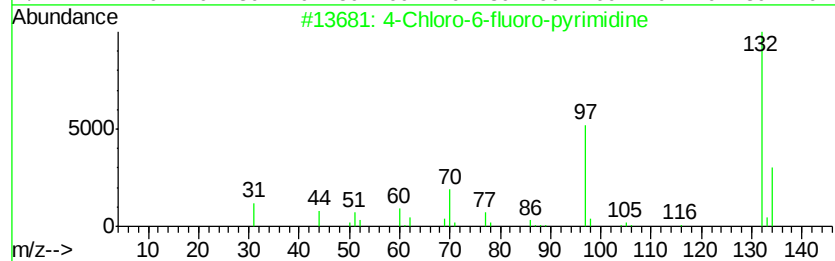
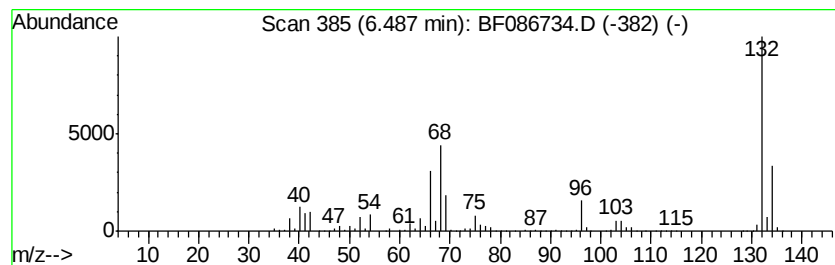
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	170.93 ng	5118710	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

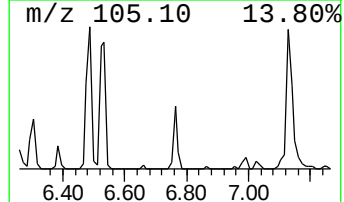
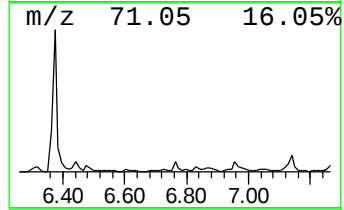
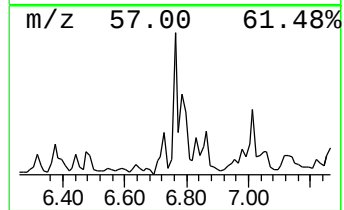
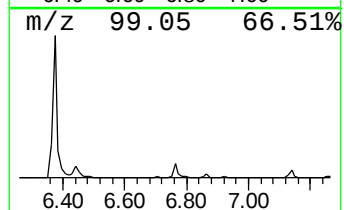
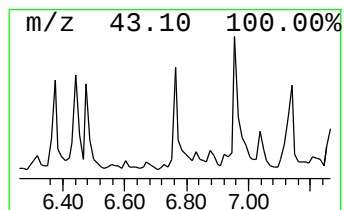
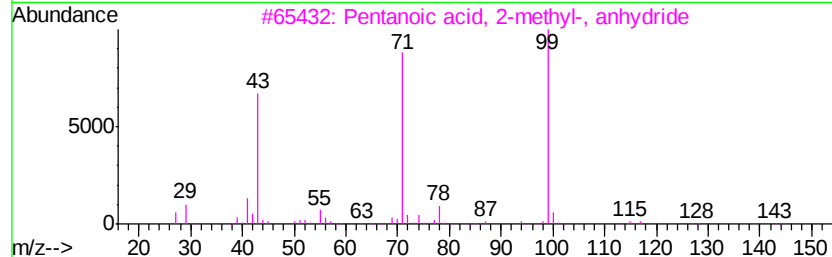
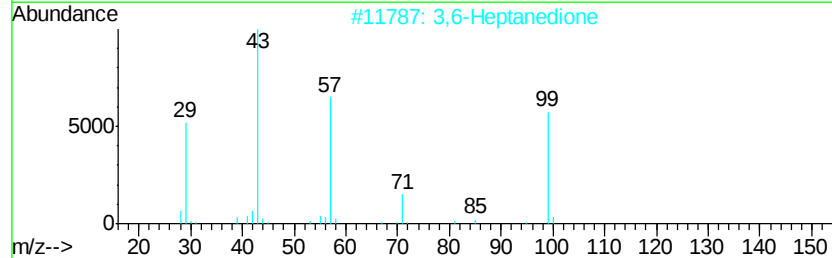
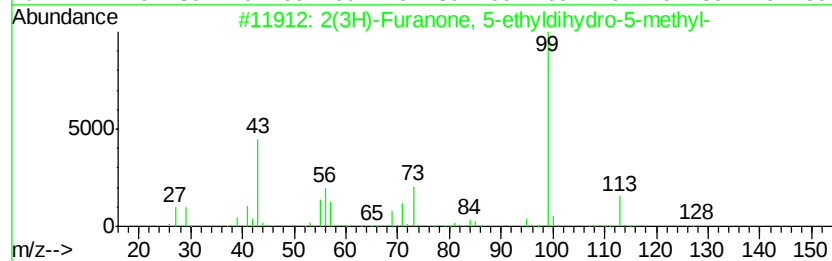
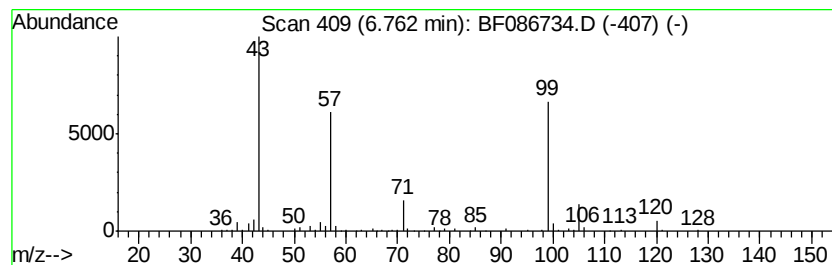
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 2(3H)-Furanone, 5-ethylidih... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	11.20 ng	335246	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, 5-ethylidihydro-5...	128	C7H12O2	002865-82-9	64
2		3,6-Heptanedione	128	C7H12O2	001703-51-1	64
3		Pentanoic acid, 2-methyl-, anhyd...	214	C12H22O3	063169-61-9	42
4		3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	42
5		Pentanoic acid, 4-oxo-, pentyl e...	186	C10H18O3	020279-49-6	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

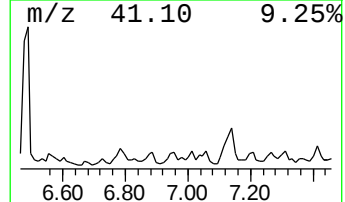
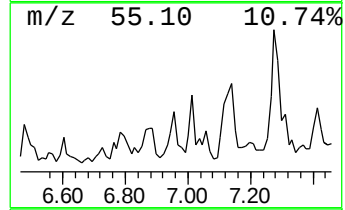
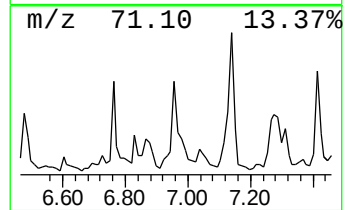
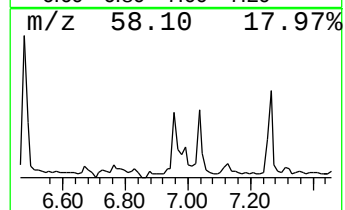
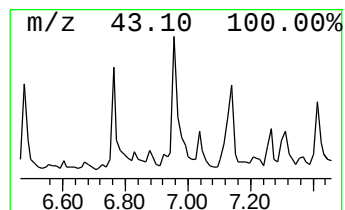
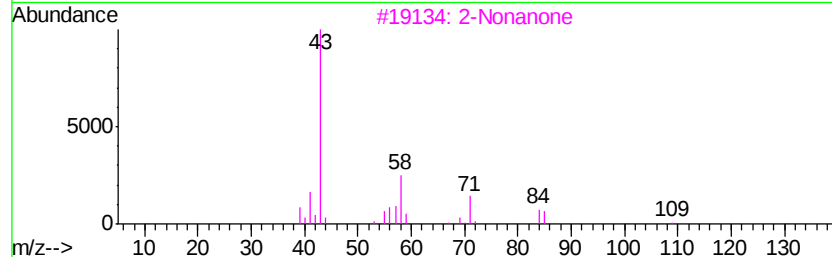
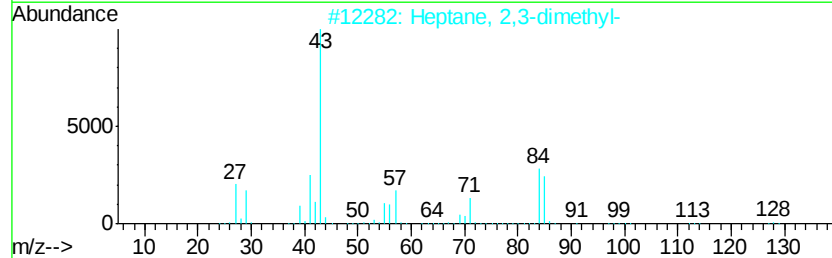
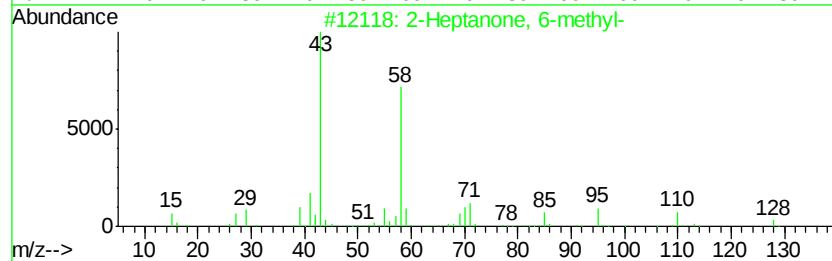
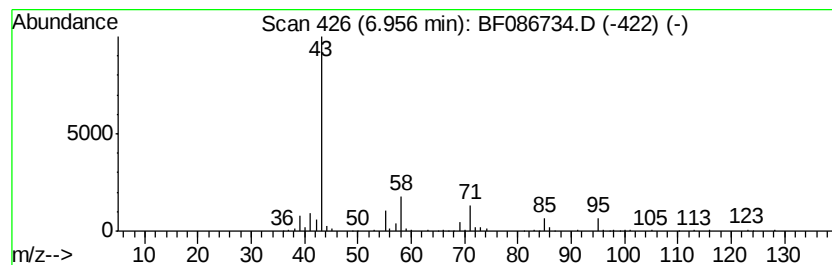
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 2-Heptanone, 6-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	10.36 ng	310276	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	59
2			Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	43
3			2-Nonanone	142	C9H18O	000821-55-6	42
4			2,9-Decanedione	170	C10H18O2	016538-91-3	40
5			Pentanal, 2-methyl-	100	C6H12O	000123-15-9	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

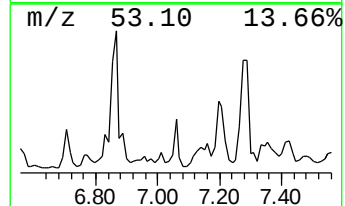
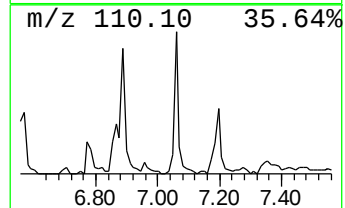
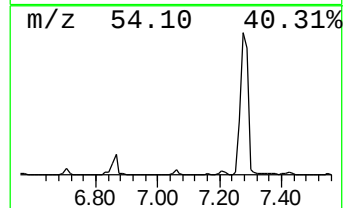
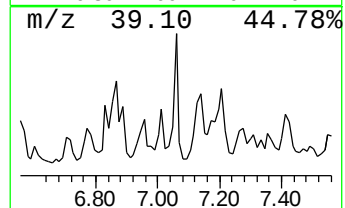
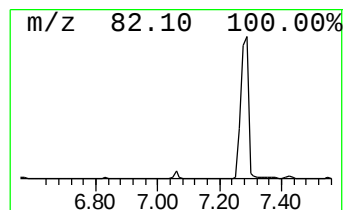
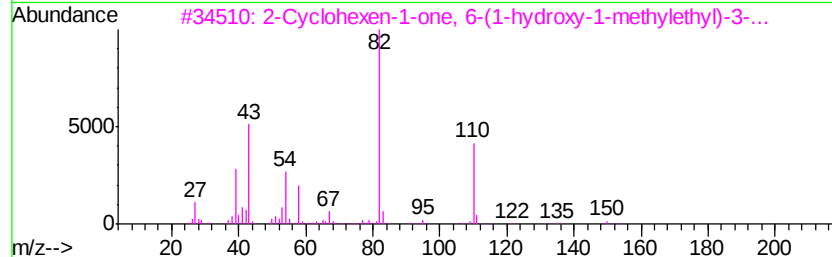
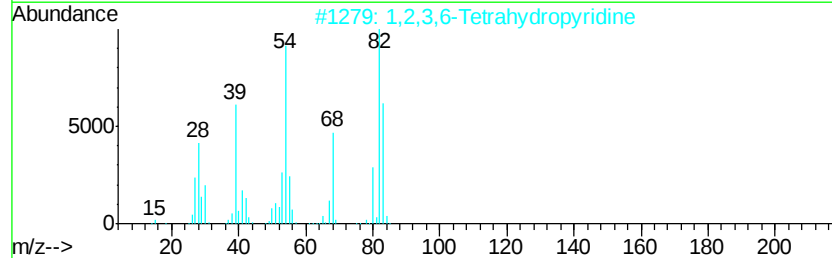
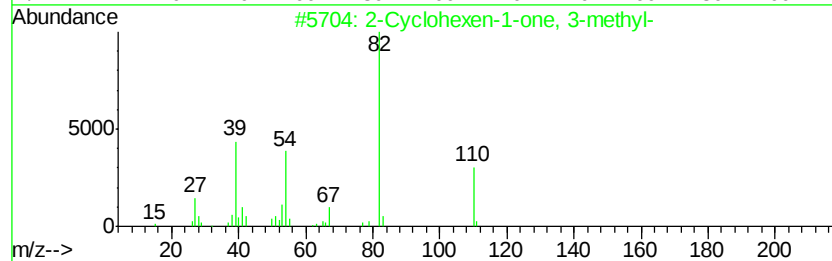
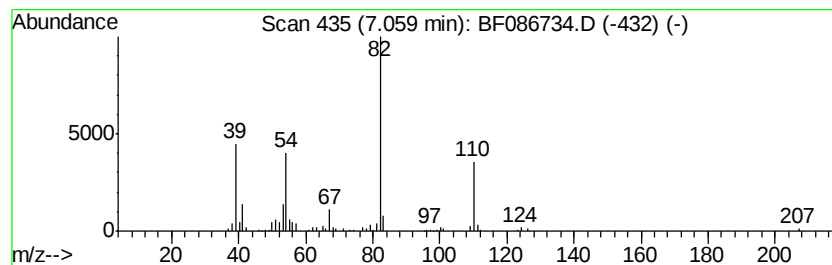
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.06	9.47 ng	283728	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2			1,2,3,6-Tetrahydropyridine	83	C5H9N	000694-05-3	50
3			2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	50
4			1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	49
5			5-Cycloheptene-1,4-dione, 2,2,5-...	166	C10H14O2	058705-37-6	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

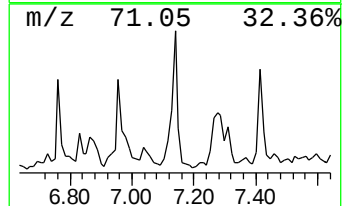
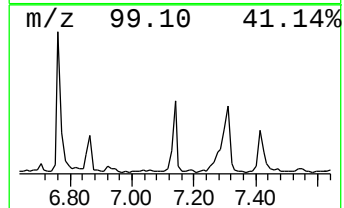
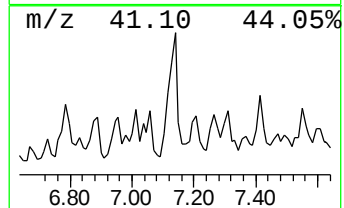
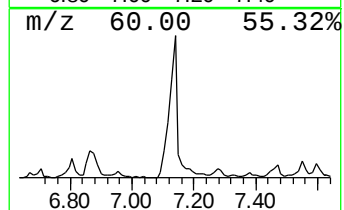
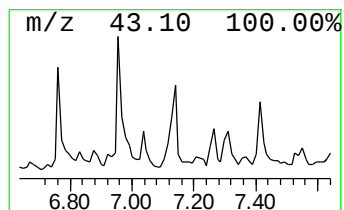
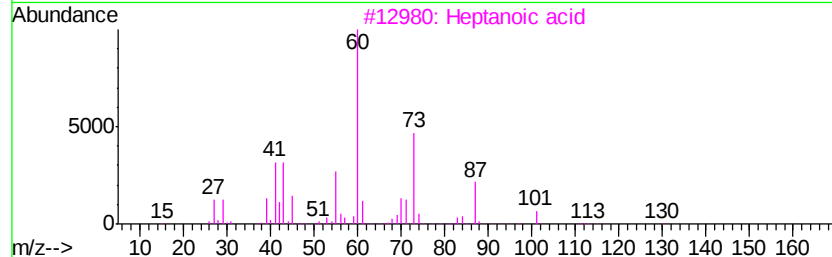
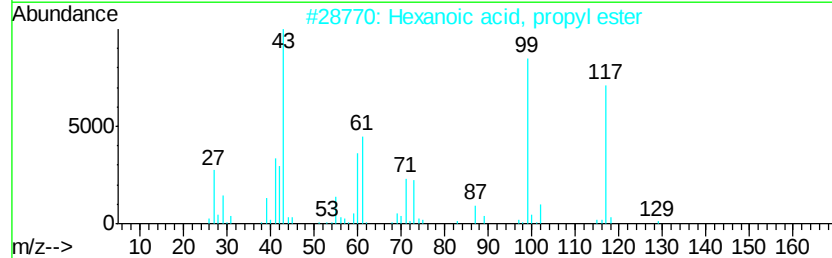
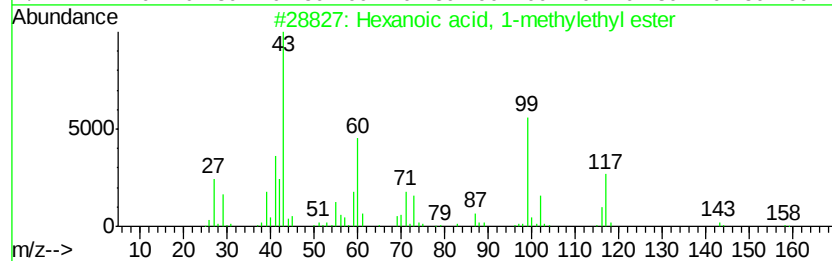
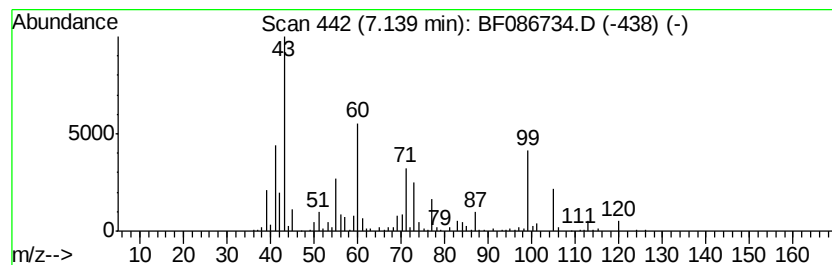
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Hexanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	22.96 ng	687512	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 1-methylethyl ester	158	C9H18O2	002311-46-8	53
2		Hexanoic acid, propyl ester	158	C9H18O2	000626-77-7	38
3		Heptanoic acid	130	C7H14O2	000111-14-8	35
4		Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	35
5		Hexanoic acid	116	C6H12O2	000142-62-1	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

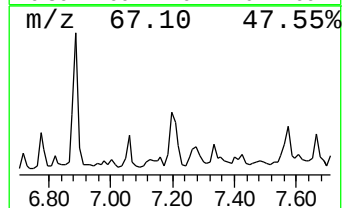
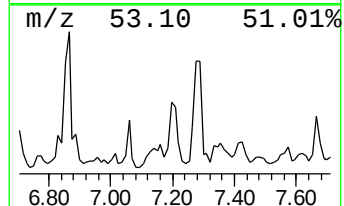
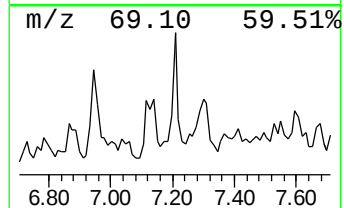
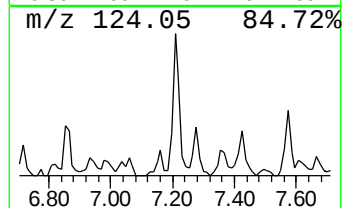
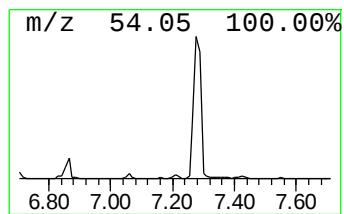
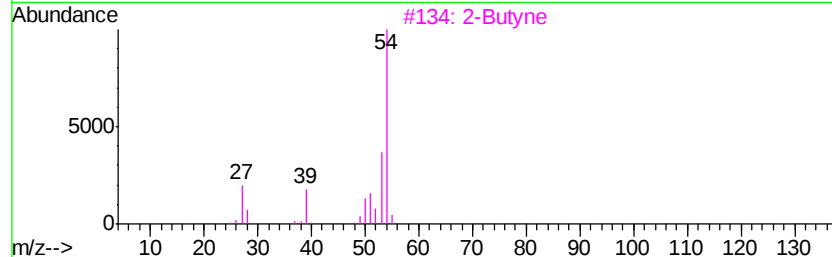
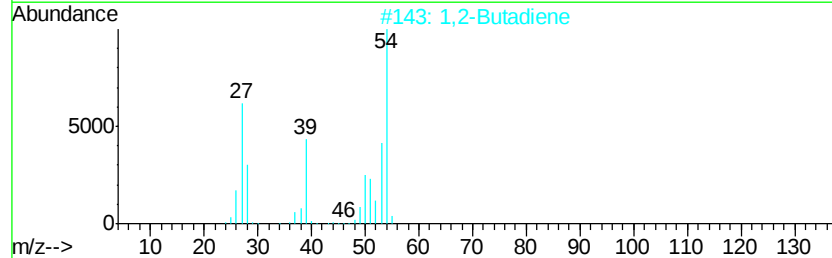
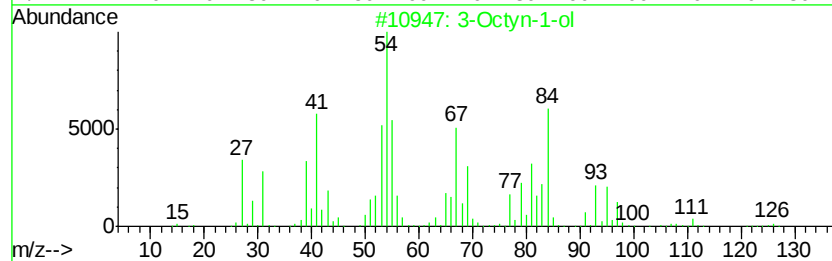
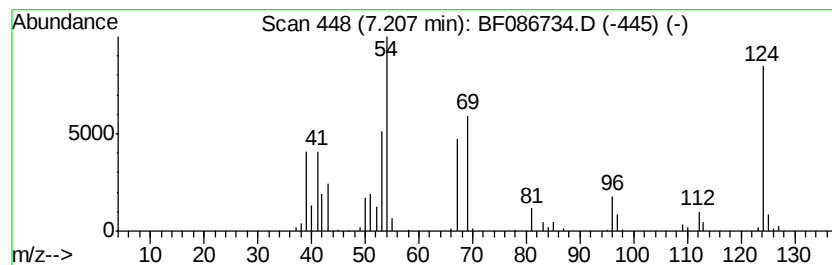
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 3-Octyn-1-ol Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	6.88 ng	206074	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octyn-1-ol	126	C8H14O	014916-80-4	53
2			1,2-Butadiene	54	C4H6	000590-19-2	53
3			2-Butyne	54	C4H6	000503-17-3	53
4			3-Pentyn-1-ol	84	C5H8O	010229-10-4	45
5			2,5-Dihydrothiophene sulfone	118	C4H6O2S	000077-79-2	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

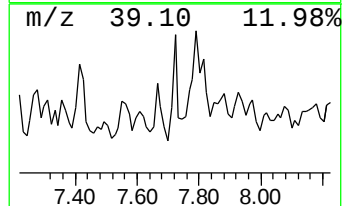
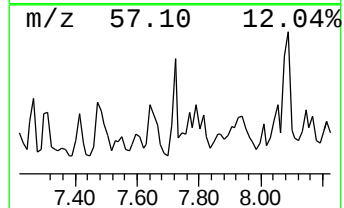
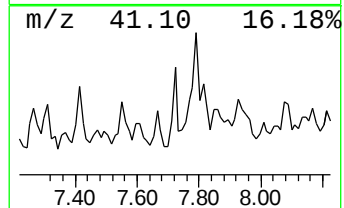
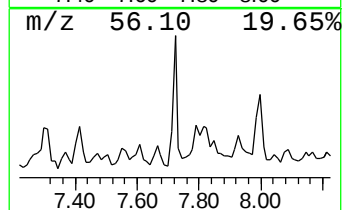
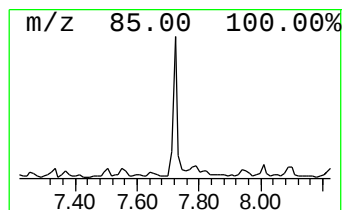
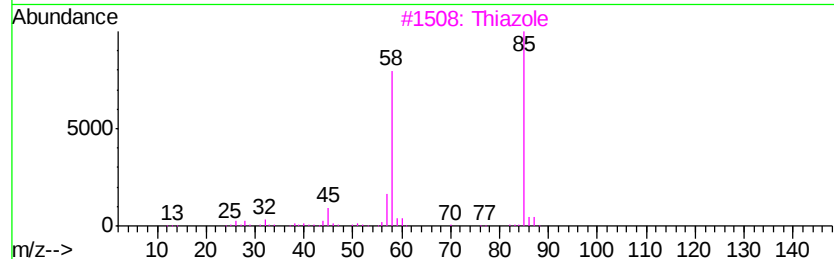
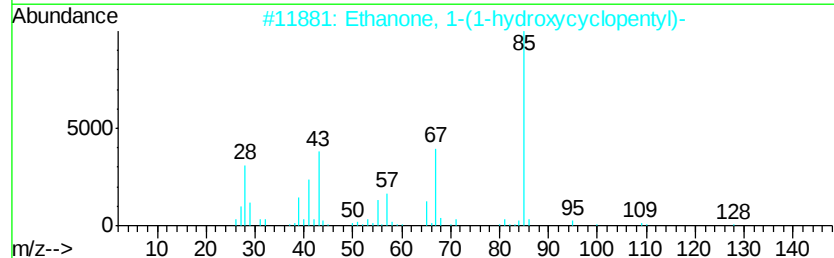
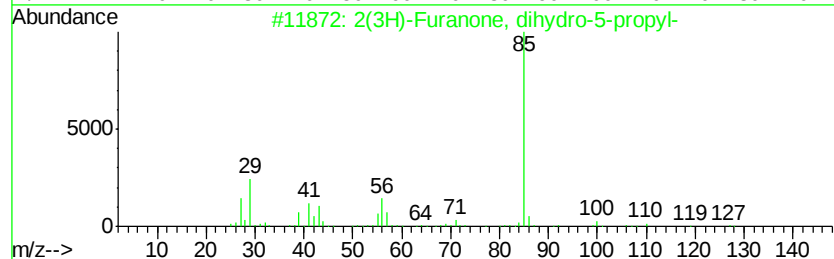
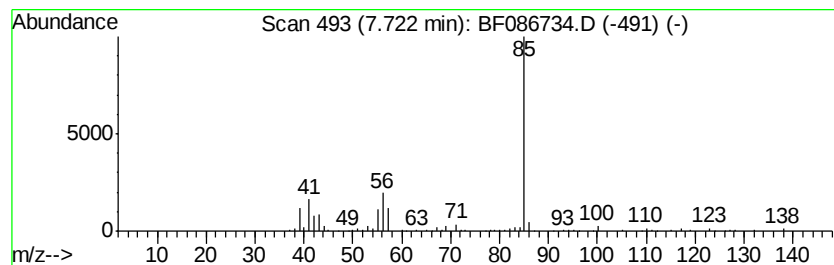
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 2(3H)-Furanone, dihydro-5-p... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.72	6.96 ng	268603	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	83
2		Ethanone, 1-(1-hydroxycyclopentyl)-	128	C7H12O2	017160-89-3	59
3		Thiazole	85	C3H3NS	000288-47-1	59
4		1-Bromo-7-(tetrahydro-2-pyranylo...	278	C12H23BrO2	010160-25-5	56
5		2-Pyrrolidinone	85	C4H7NO	000616-45-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

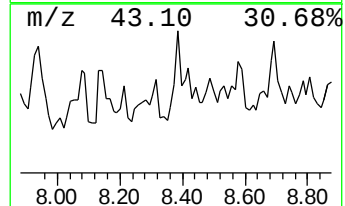
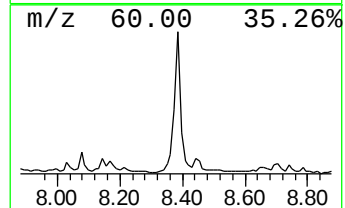
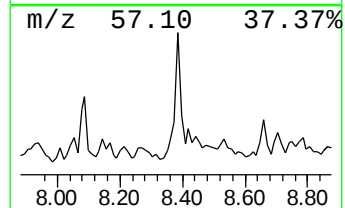
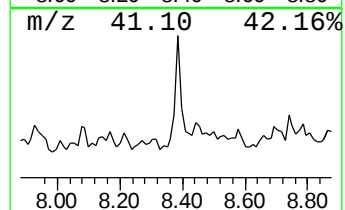
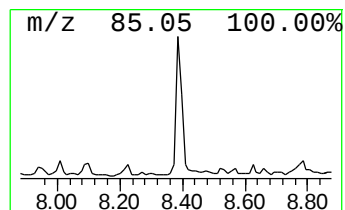
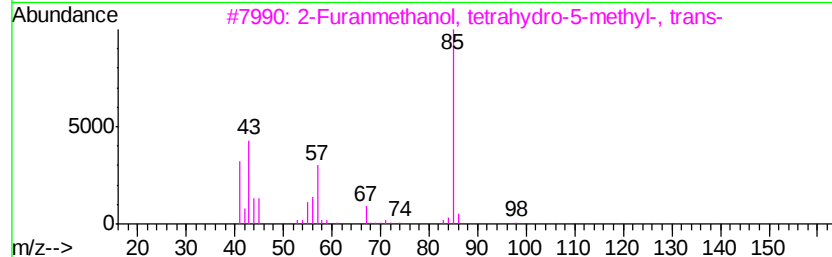
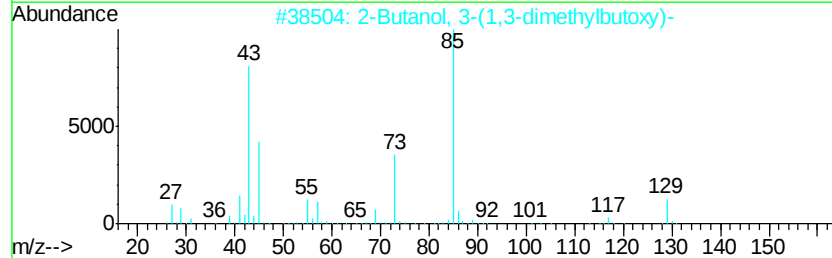
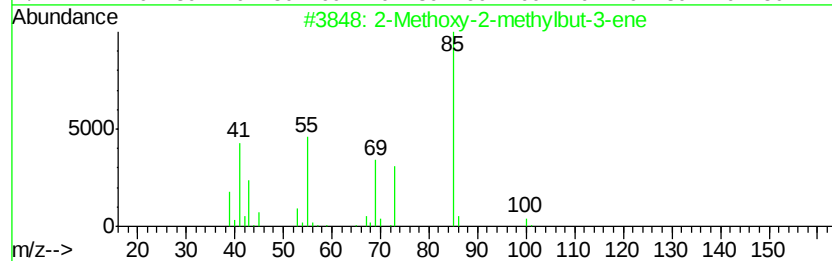
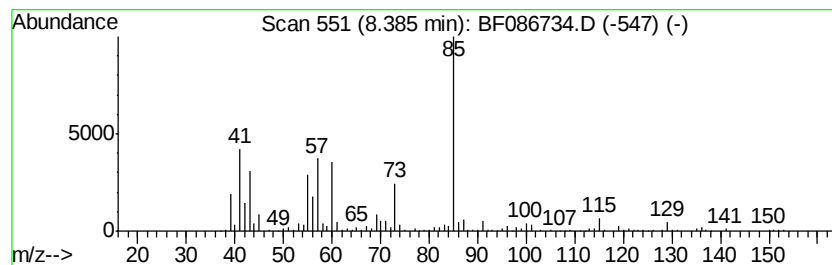
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 2-Methoxy-2-methylbut-3-ene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	17.66 ng	682039	Napthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Methoxy-2-methylbut-3-ene	100	C6H12O	040426-44-6	58
2		2-Butanol, 3-(1,3-dimethylbutoxy)-	174	C10H22O2	074810-45-0	53
3		2-Furanmethanol, tetrahydro-5-me...	116	C6H12O2	054774-28-6	47
4		2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2	000706-14-9	47
5		2H-Pyran, tetrahydro-2-(12-penta...	308	C20H36O2	056666-38-7	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

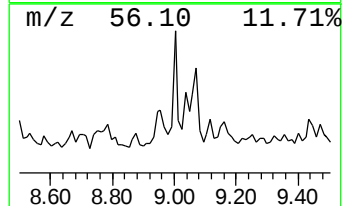
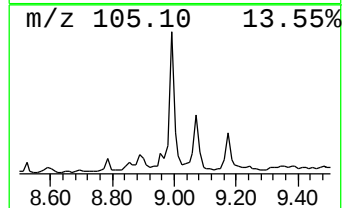
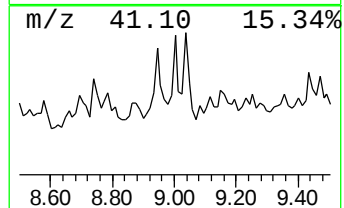
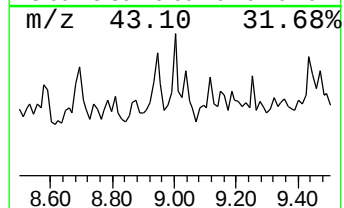
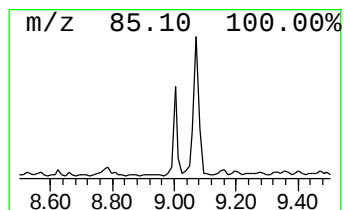
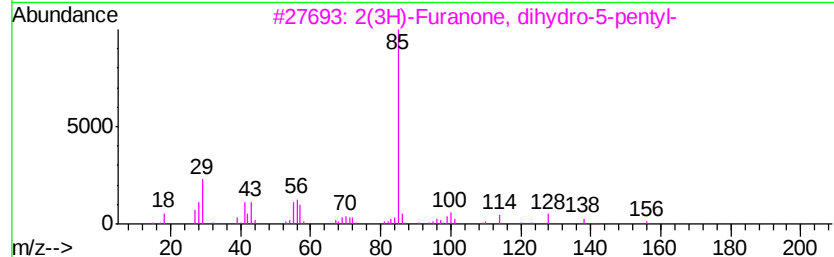
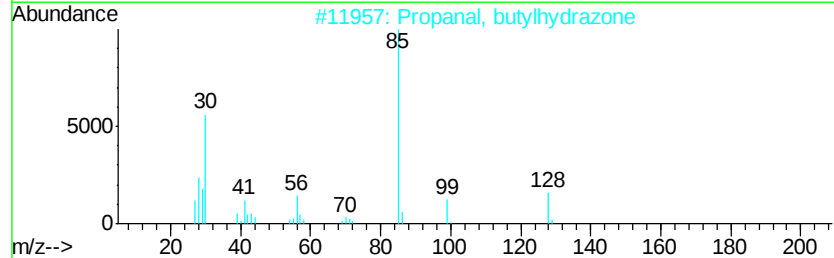
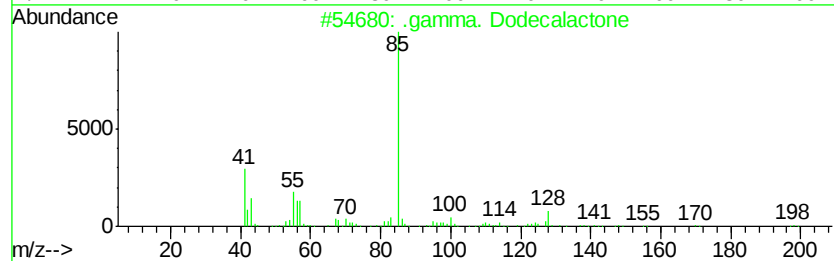
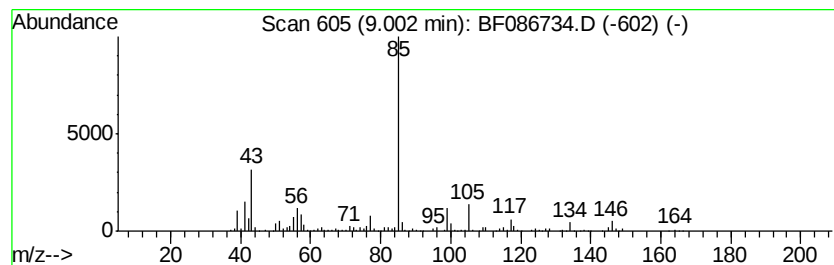
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 .gamma. Dodecalactone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.00	11.14 ng	495687	Acenaphthene-d10	9.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.gamma. Dodecalactone	198	C12H22O2	002305-05-7	59
2		Propanal, butylhydrazone	128	C7H16N2	020607-75-4	59
3		2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	59
4		2-Pyrrolidinone	85	C4H7NO	000616-45-5	58
5		2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

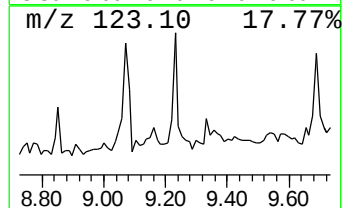
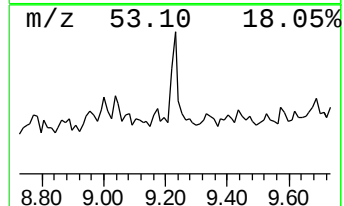
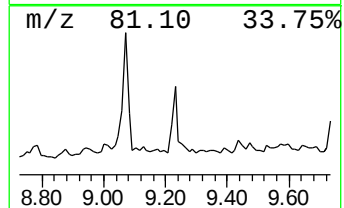
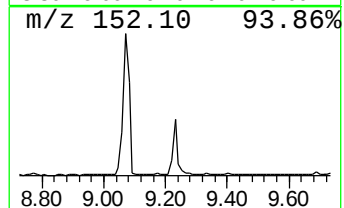
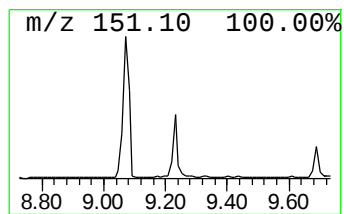
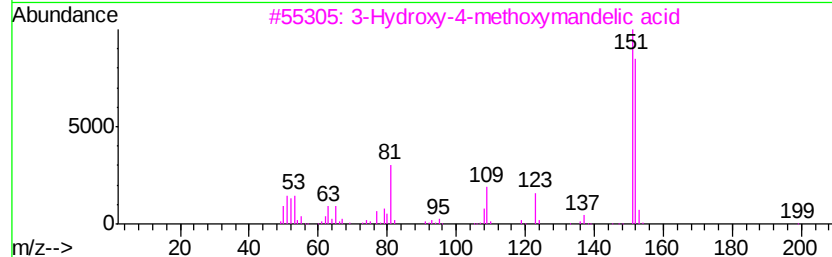
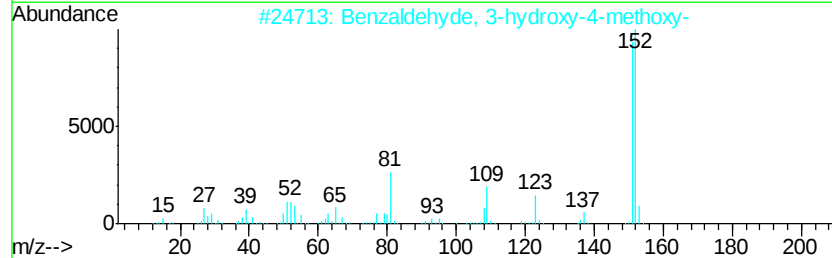
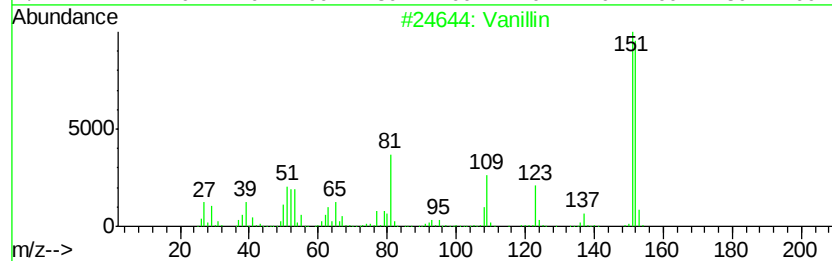
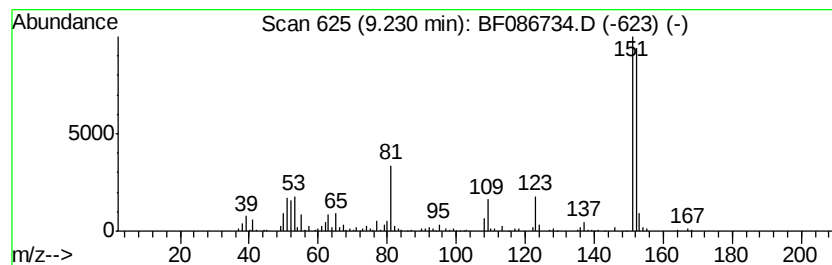
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Vanillin Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.23	7.51 ng	333928	Acenaphthene-d10	9.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin	152	C8H8O3	000121-33-5	95
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	95
3			3-Hydroxy-4-methoxymandelic acid	198	C9H10O5	003695-24-7	91
4			4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	90
5			Benzaldehyde, 4-(methylthio)-	152	C8H8OS	003446-89-7	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

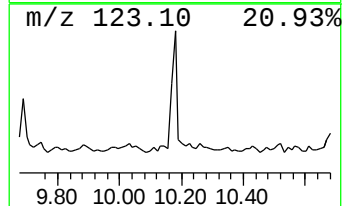
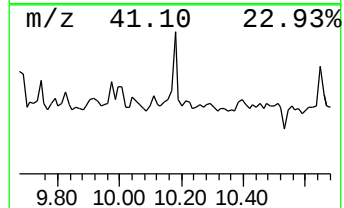
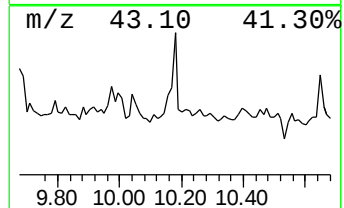
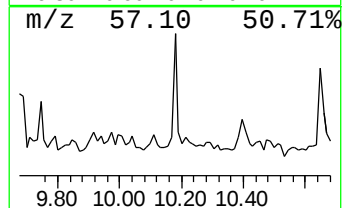
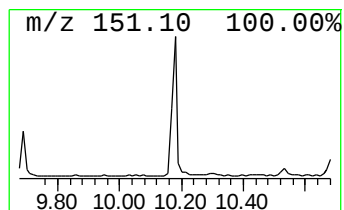
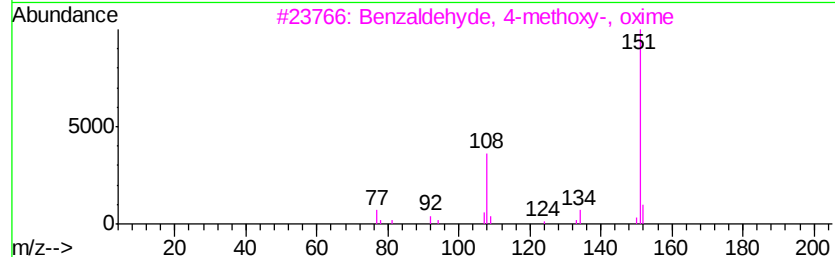
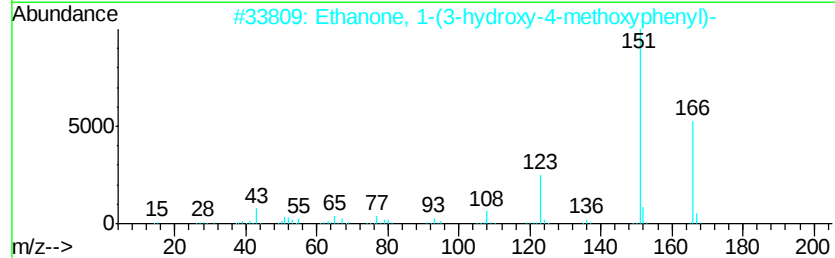
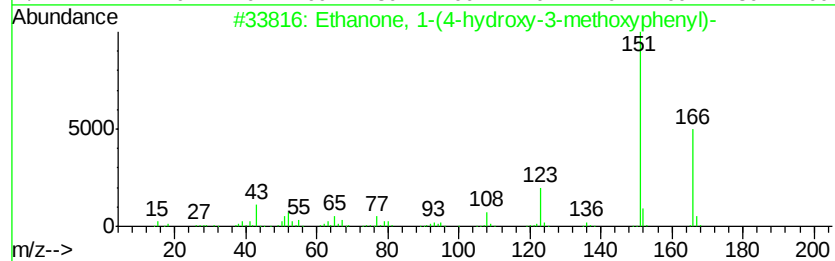
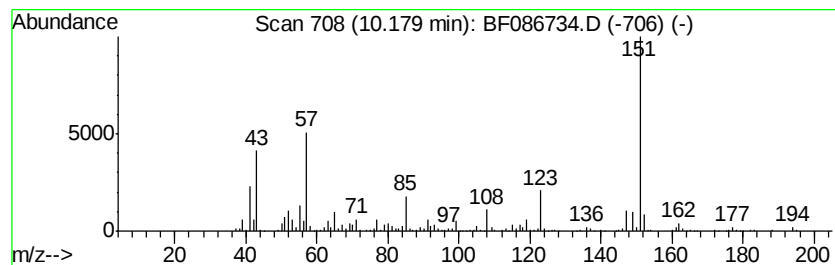
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Ethanone, 1-(4-hydroxy-3-me... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	7.04 ng	313332	Acenaphthene-d10	9.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(4-hydroxy-3-methoxy...	166	C9H10O3	000498-02-2	53
2			Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	53
3			Benzaldehyde, 4-methoxy-, oxime	151	C8H9NO2	003235-04-9	47
4			7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	47
5			Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

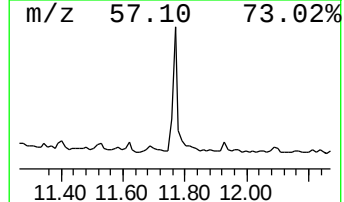
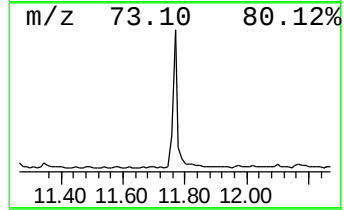
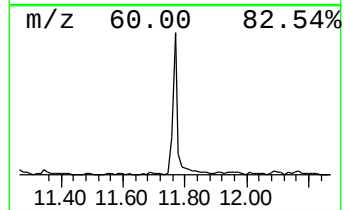
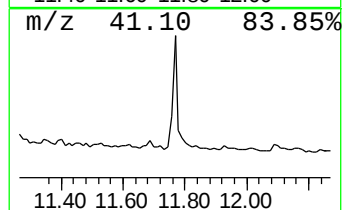
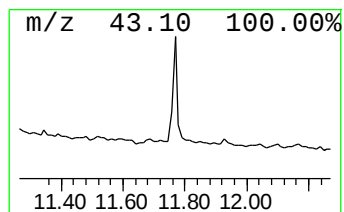
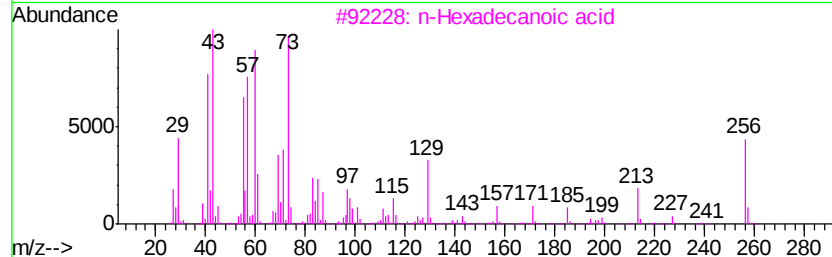
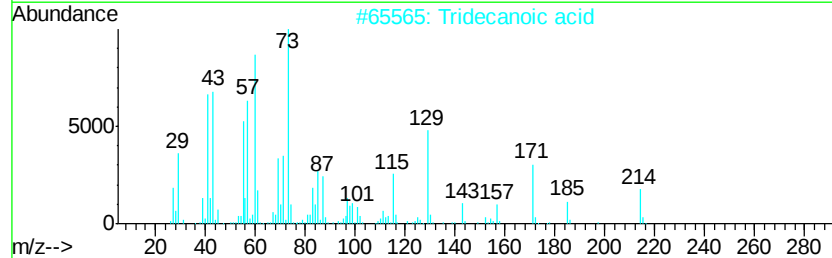
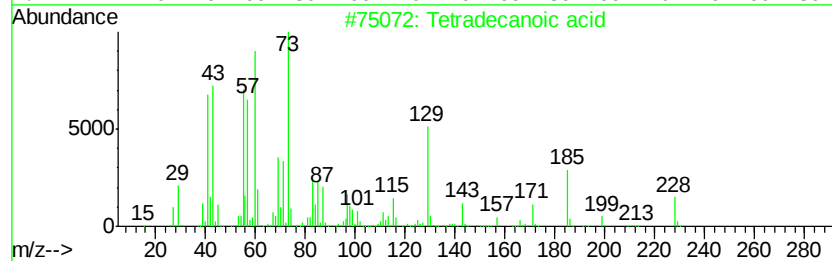
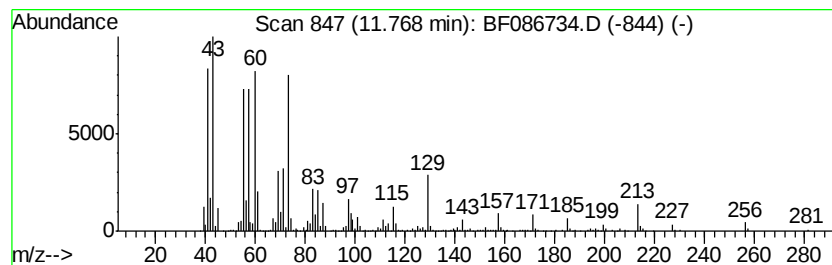
Instrument :
BNA_F
ClientSampleId :
MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.77	11.30 ng	409688	Phenanthrene-d10		11.22
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
5	Undecanoic acid	186	C11H22O2	000112-37-8	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
Data File : BF086734.D
Acq On : 6 May 2016 20:04
Operator : UM/SJ
Sample : H2802-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-3

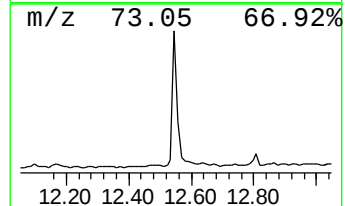
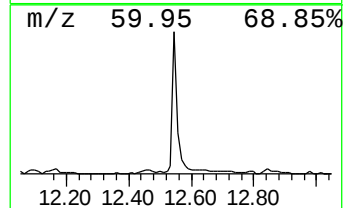
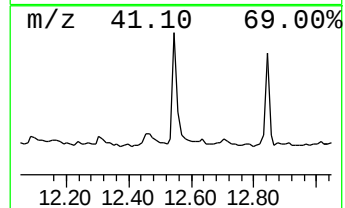
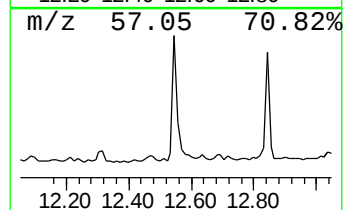
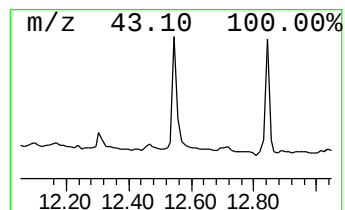
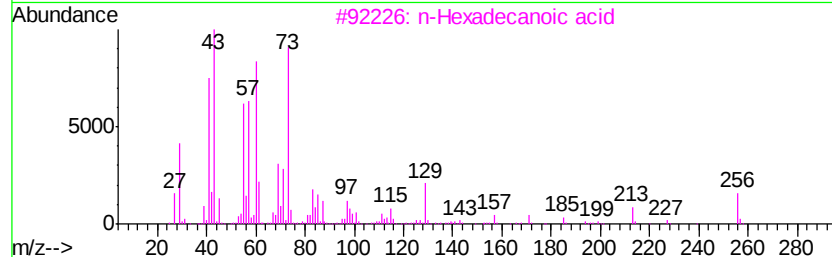
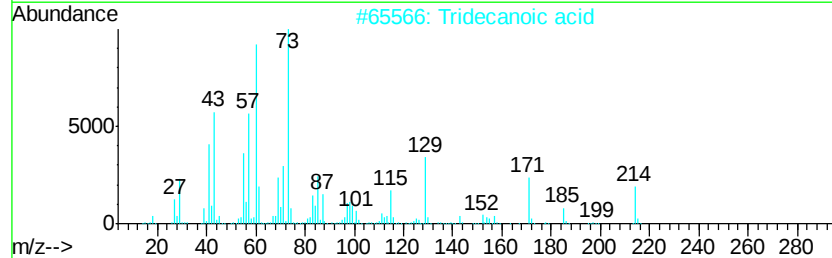
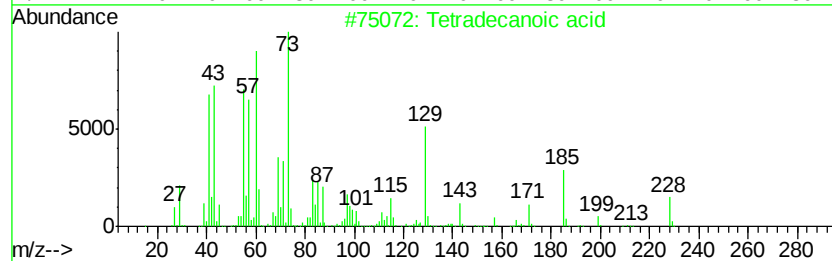
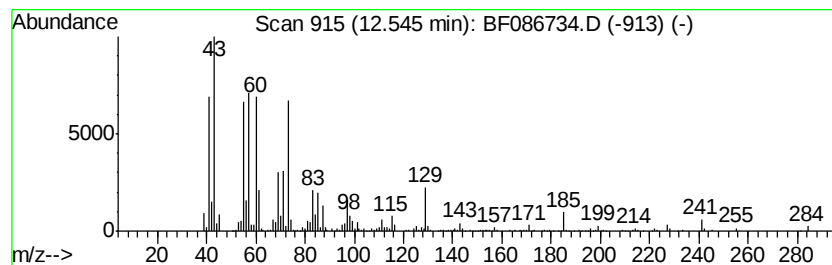
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	12.06 ng	363930	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5		n-Decanoic acid	172	C10H20O2	000334-48-5	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050616\
 Data File : BF086734.D
 Acq On : 6 May 2016 20:04
 Operator : UM/SJ
 Sample : H2802-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050416.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Heptanone	5.49	9.1 ng		272206	1	6.70	1197840	40.0
2,5-Hexanedione	5.89	9.3 ng		277568	1	6.70	1197840	40.0
unknown6.14	6.14	16.6 ng		495735	1	6.70	1197840	40.0
2-Cyclopenten-1-o...	6.30	9.8 ng		294889	1	6.70	1197840	40.0
2(3H)-Furanone, d...	6.44	16.7 ng		499034	1	6.70	1197840	40.0
unknown6.49	6.49	170.9 ng		5118710	1	6.70	1197840	40.0
2(3H)-Furanone, 5...	6.76	11.2 ng		335246	1	6.70	1197840	40.0
2-Heptanone, 6-me...	6.96	10.4 ng		310276	1	6.70	1197840	40.0
2-Cyclohexen-1-on...	7.06	9.5 ng		283728	1	6.70	1197840	40.0
Hexanoic acid, 1-...	7.14	23.0 ng		687512	1	6.70	1197840	40.0
3-Octyn-1-ol	7.21	6.9 ng		206074	1	6.70	1197840	40.0
2(3H)-Furanone, d...	7.72	7.0 ng		268603	2	8.00	1544440	40.0
2-Methoxy-2-methy...	8.38	17.7 ng		682039	2	8.00	1544440	40.0
.gamma. Dodecalac...	9.00	11.1 ng		495687	3	9.74	1779640	40.0
Vanillin	9.23	7.5 ng		333928	3	9.74	1779640	40.0
Ethanone, 1-(4-hy...	10.18	7.0 ng		313332	3	9.74	1779640	40.0
Tetradecanoic acid	11.77	11.3 ng		409688	4	11.22	1449990	40.0
Tridecanoic acid	12.55	12.1 ng		363930	5	13.85	1207130	40.0