

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
 Data File : BF088677.D
 Acq On : 4 Jul 2016 6:19
 Operator : UM/SJ
 Sample : H3784-02
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D10-B2(0-11)C

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-BF063016.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	1.724	10	12	19	rVV2	23836	38179	1.34%	0.132%
2	1.850	21	23	34	rVV	244778	365996	12.82%	1.267%
3	2.010	34	37	51	rVB2	21329	54976	1.93%	0.190%
4	4.947	292	294	299	rBB	123453	180821	6.33%	0.626%
5	5.382	329	332	334	rBV	2279769	2706067	94.78%	9.369%
6	5.599	349	351	353	rBV	57160	58330	2.04%	0.202%
7	6.422	420	423	425	rVB	2374504	2855223	100.00%	9.885%
8	6.547	431	434	437	rBV	2371640	2448719	85.76%	8.478%
9	6.616	438	440	442	rBV2	44134	52750	1.85%	0.183%
10	6.787	452	455	456	rBV	531623	686452	24.04%	2.377%
11	6.936	466	468	471	rVB	1898894	1961976	68.72%	6.792%
12	7.050	476	478	482	rBB2	26513	43353	1.52%	0.150%
13	7.348	501	504	506	rBV	1808975	1803088	63.15%	6.242%
14	7.645	527	530	532	rBV	61751	55102	1.93%	0.191%
15	8.068	565	567	569	rBV	1188986	1009721	35.36%	3.496%
16	8.342	589	591	593	rVB	53073	42486	1.49%	0.147%
17	9.142	658	661	664	rVB	2560467	2586184	90.58%	8.953%
18	9.268	670	672	674	rBV	46923	43322	1.52%	0.150%
19	9.531	694	695	698	rVB	183995	248447	8.70%	0.860%
20	9.759	713	715	718	rBV2	32462	30643	1.07%	0.106%
21	9.816	718	720	722	rVV	1224754	1044471	36.58%	3.616%
22	10.262	757	759	760	rVB	33175	28765	1.01%	0.100%
23	10.605	786	789	791	rBV	1363103	1729334	60.57%	5.987%
24	10.731	798	800	803	rBV	48234	52841	1.85%	0.183%
25	11.176	837	839	845	rVB2	100355	117384	4.11%	0.406%
26	11.291	847	849	853	rVV2	1165333	1244548	43.59%	4.309%
27	11.359	853	855	857	rVB2	50696	71570	2.51%	0.248%
28	11.599	874	876	879	rVB2	35931	47117	1.65%	0.163%
29	11.794	891	893	894	rBV	42342	38149	1.34%	0.132%
30	11.817	894	895	898	rVV	58033	59426	2.08%	0.206%
31	11.897	901	902	907	rVB2	58758	92441	3.24%	0.320%
32	11.988	908	910	916	rVB4	13512	30362	1.06%	0.105%
33	12.102	916	920	924	rBV2	37946	65796	2.30%	0.228%
34	12.342	938	941	942	rBV	25210	33148	1.16%	0.115%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
 Data File : BF088677.D
 Acq On : 4 Jul 2016 6:19
 Operator : UM/SJ
 Sample : H3784-02
 Misc :
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D10-B2(0-11)C

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-BF063016.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.422	945	948	950	rVV3	23033	42244	1.48%	0.146%
36	12.491	952	954	957	rVV	289307	377884	13.23%	1.308%
37	12.719	971	974	977	rBV2	450075	581707	20.37%	2.014%
38	12.788	977	980	982	rVB3	42995	61618	2.16%	0.213%
39	12.879	985	988	990	rVB	2547197	2465188	86.34%	8.535%
40	12.948	990	994	997	rVB2	24559	50924	1.78%	0.176%
41	13.051	997	1003	1005	rVB3	41338	75573	2.65%	0.262%
42	13.120	1005	1009	1010	rBV	45095	45212	1.58%	0.157%
43	13.154	1010	1012	1013	rBV	49477	49985	1.75%	0.173%
44	13.417	1033	1035	1037	rBV	136296	135537	4.75%	0.469%
45	13.462	1037	1039	1040	rVV	37975	45951	1.61%	0.159%
46	13.554	1044	1047	1049	rBV	32213	42481	1.49%	0.147%
47	13.668	1054	1057	1058	rBV2	24210	35262	1.23%	0.122%
48	13.817	1066	1070	1075	rVB3	47975	136016	4.76%	0.471%
49	13.920	1075	1079	1080	rBV2	603413	918872	32.18%	3.181%
50	14.022	1084	1088	1090	rBV2	15311	30137	1.06%	0.104%
51	14.102	1093	1095	1096	rBV	53009	44613	1.56%	0.154%
52	14.297	1110	1112	1114	rBV	28663	31878	1.12%	0.110%
53	14.411	1119	1122	1124	rBV2	40692	64587	2.26%	0.224%
54	14.697	1146	1147	1150	rVB2	34823	46660	1.63%	0.162%
55	14.914	1164	1166	1171	rBV	150438	272614	9.55%	0.944%
56	15.017	1173	1175	1177	rVB	53083	66344	2.32%	0.230%
57	15.097	1177	1182	1185	rBV4	13462	48535	1.70%	0.168%
58	15.188	1188	1190	1193	rVB	97088	103249	3.62%	0.357%
59	15.245	1193	1195	1198	rBV	113417	133505	4.68%	0.462%
60	15.303	1198	1200	1203	rBV	482701	666358	23.34%	2.307%
61	15.760	1237	1240	1243	rBV2	22829	43587	1.53%	0.151%
62	16.480	1299	1303	1310	rVV4	15978	42965	1.50%	0.149%
63	16.628	1313	1316	1321	rVB2	57688	107374	3.76%	0.372%
64	17.028	1348	1351	1357	rVB	47197	103829	3.64%	0.359%
65	17.234	1366	1369	1376	rVB2	12581	36338	1.27%	0.126%
66	19.052	1524	1528	1536	rVB2	13018	50488	1.77%	0.175%

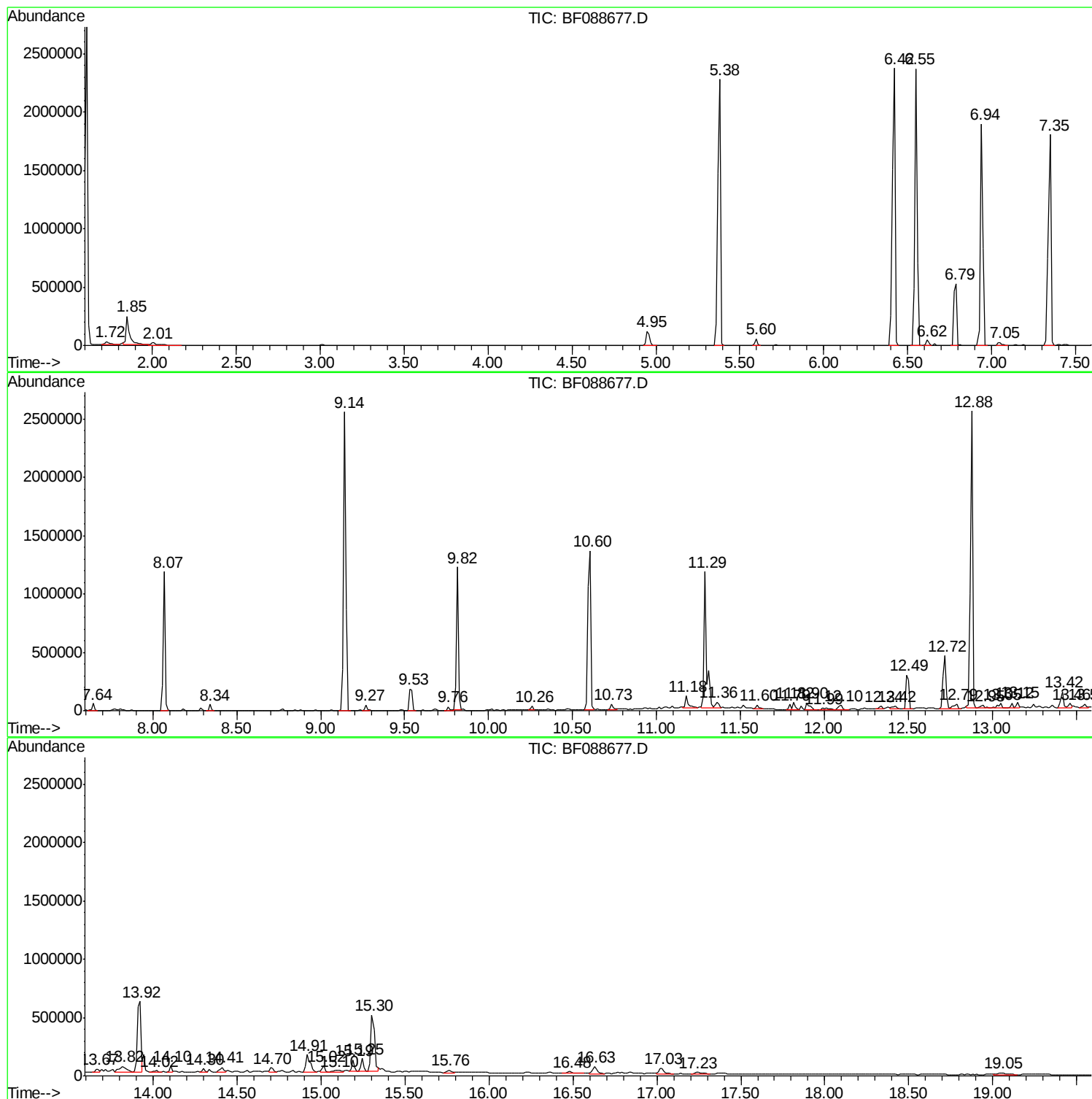
Sum of corrected areas: 28884702

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088677.D
Acq On : 4 Jul 2016 6:19
Operator : UM/SJ
Sample : H3784-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D10-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088677.D
Acq On : 4 Jul 2016 6:19
Operator : UM/SJ
Sample : H3784-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D10-B2(0-11)C

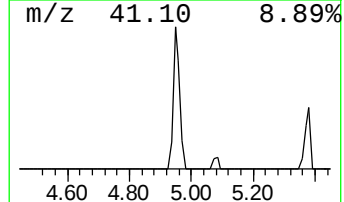
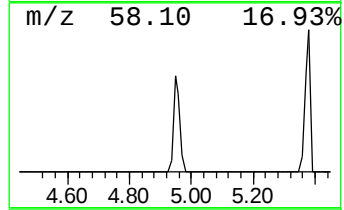
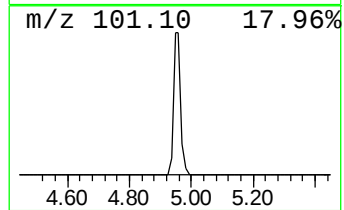
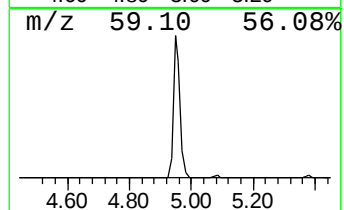
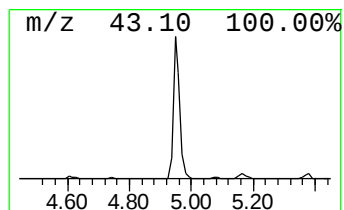
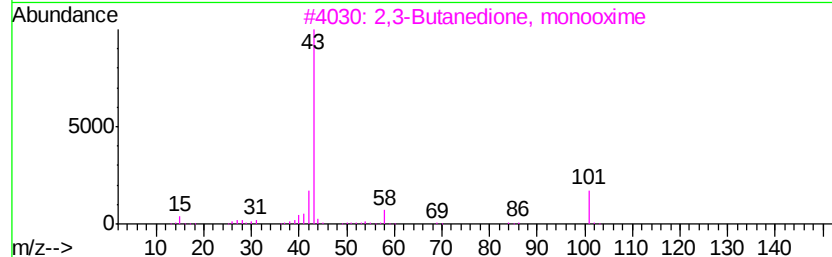
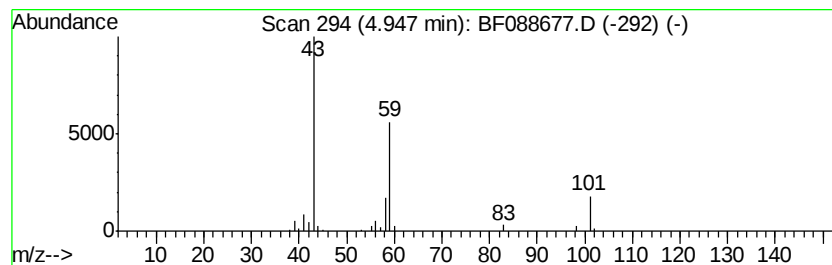
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	5.27 ng	180821	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088677.D
Acq On : 4 Jul 2016 6:19
Operator : UM/SJ
Sample : H3784-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D10-B2(0-11)C

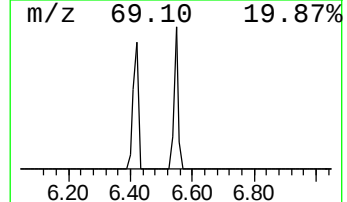
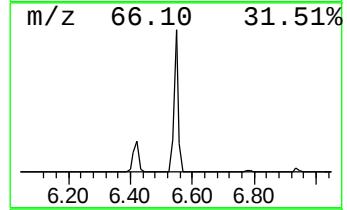
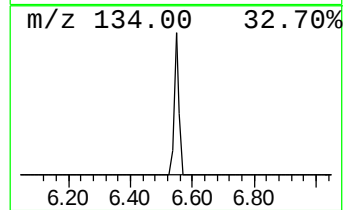
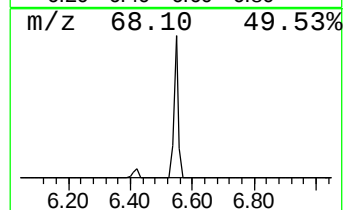
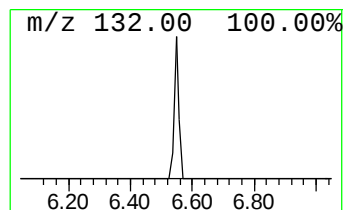
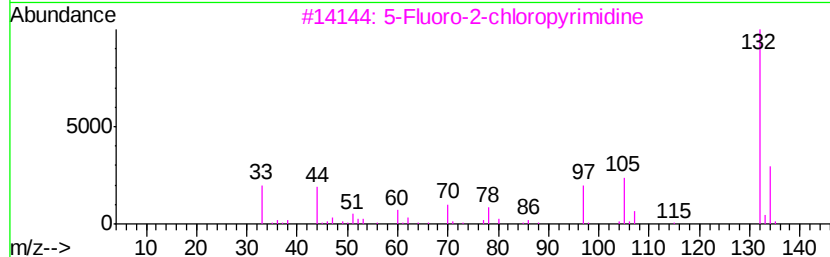
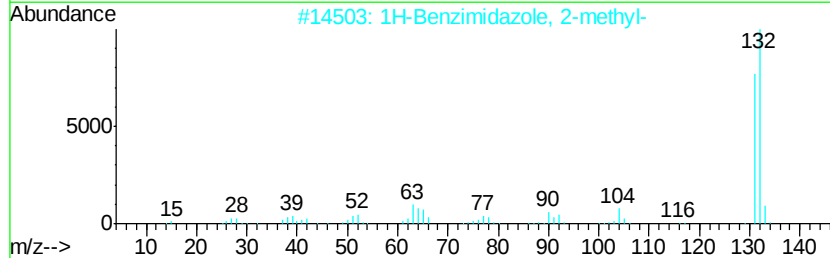
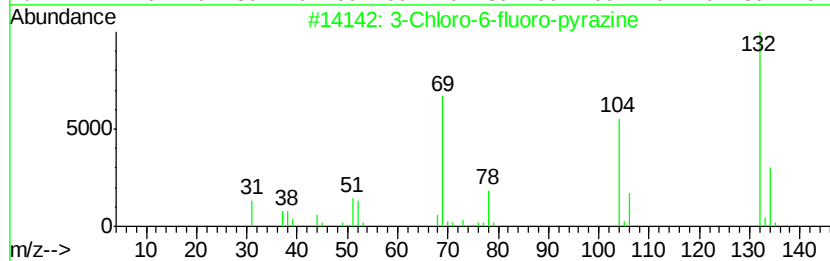
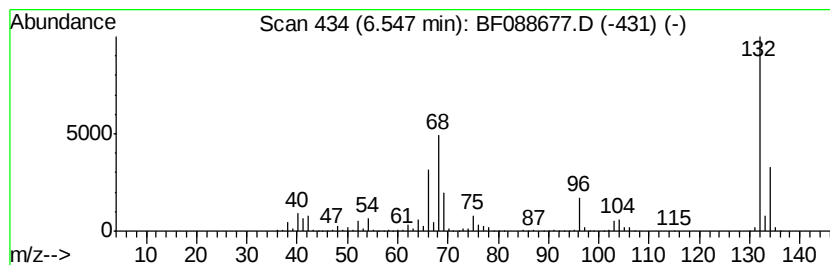
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	71.34 ng	2448720	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4			(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5			Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088677.D
Acq On : 4 Jul 2016 6:19
Operator : UM/SJ
Sample : H3784-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D10-B2(0-11)C

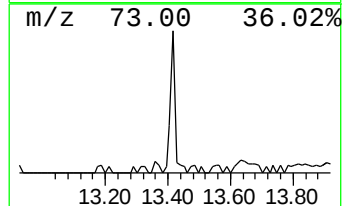
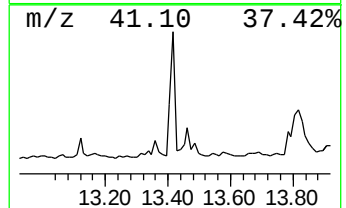
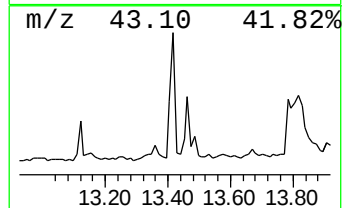
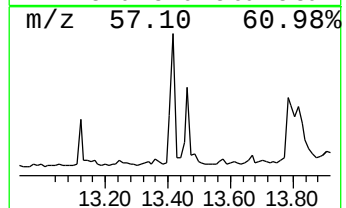
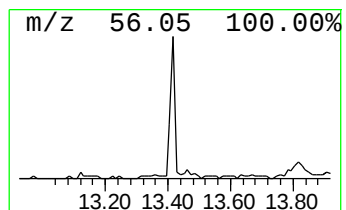
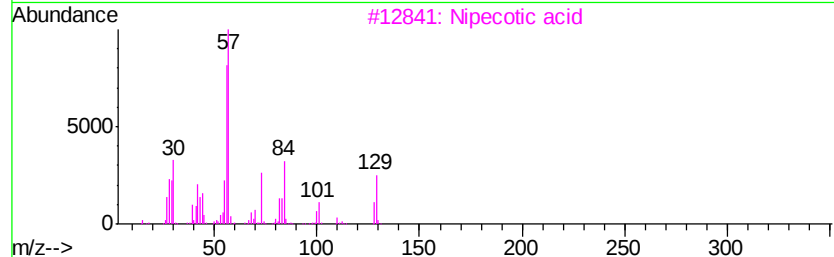
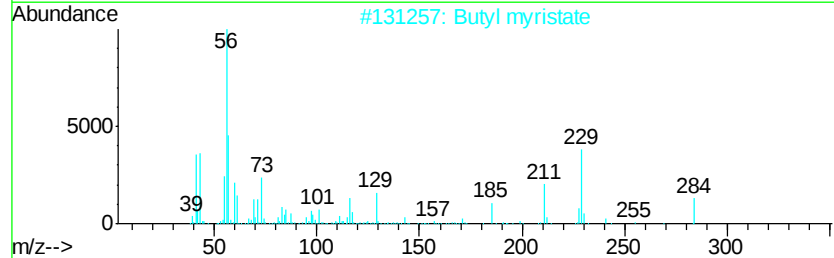
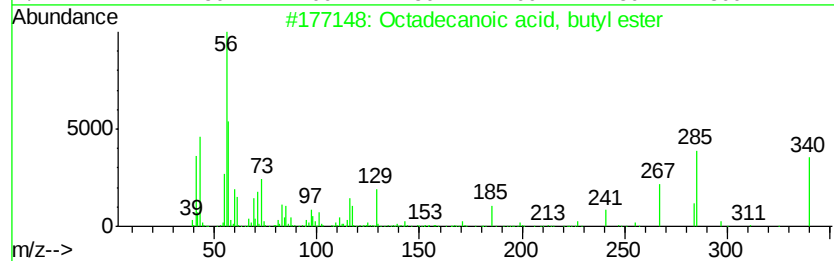
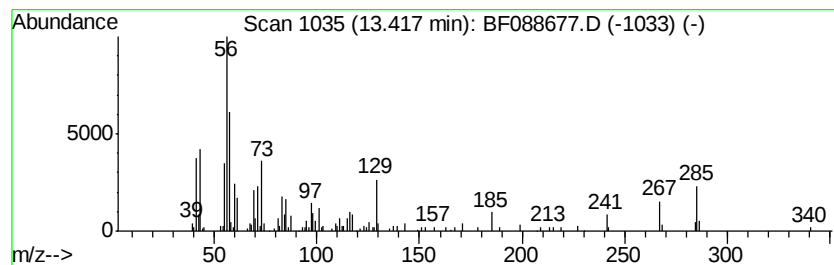
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	2.95 ng	135537	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	87
2		Butyl myristate	284	C18H36O2	000110-36-1	53
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	38
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088677.D
Acq On : 4 Jul 2016 6:19
Operator : UM/SJ
Sample : H3784-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D10-B2(0-11)C

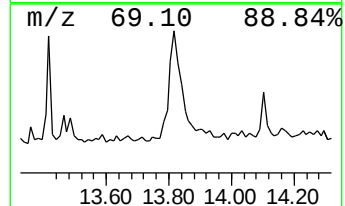
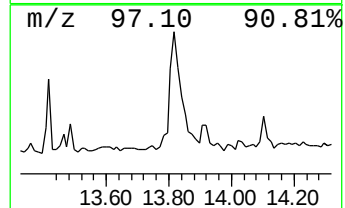
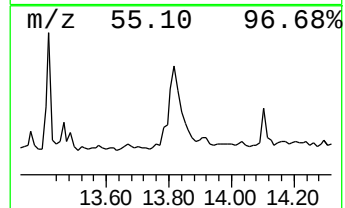
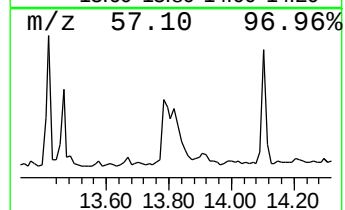
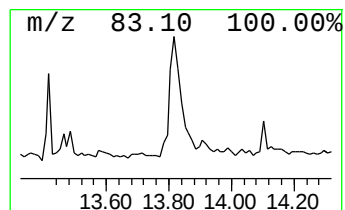
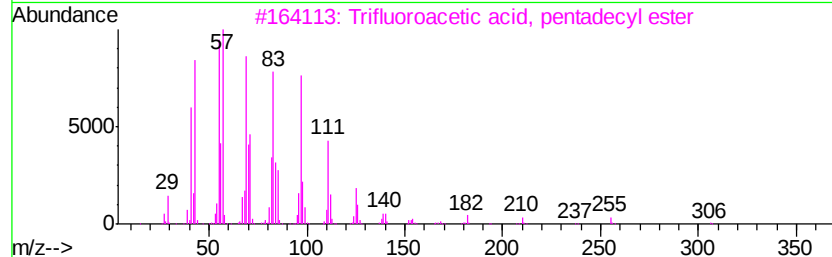
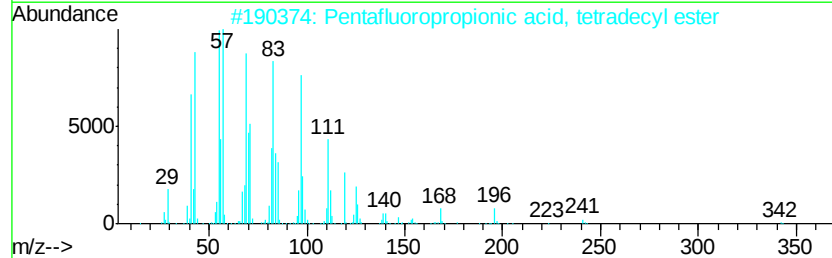
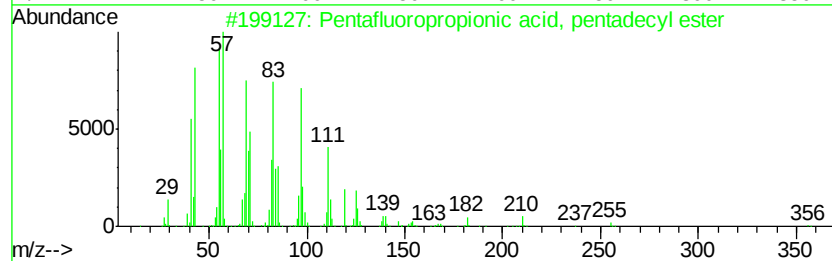
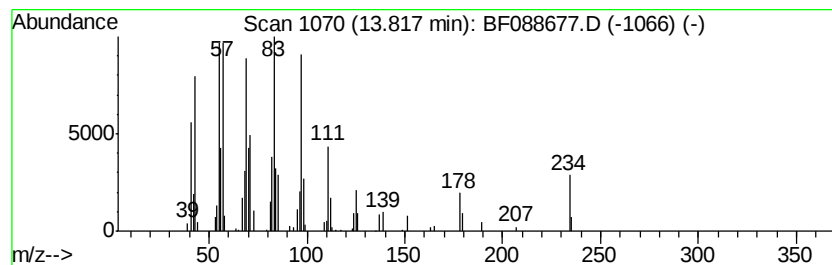
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.96 ng	136016	Chrysene-d12	13.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
2		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	93
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5		Behenic alcohol	326	C22H46O	000661-19-8	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088677.D
Acq On : 4 Jul 2016 6:19
Operator : UM/SJ
Sample : H3784-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D10-B2(0-11)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
2-Pentanone, 4-hy...	4.95	5.3	ng	180821	1	6.79	686452	20.0
unknown6.55	6.55	71.3	ng	2448720	1	6.79	686452	20.0
Octadecanoic acid...	13.42	3.0	ng	135537	5	13.92	918872	20.0
Pentafluoropropio...	13.82	3.0	ng	136016	5	13.92	918872	20.0