

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
 Data File : BF088310.D
 Acq On : 24 Jun 2016 1:34
 Operator : UM/SJ
 Sample : H3682-05
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-3(0-6)

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-BF060716.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	48	rVB	1089029	2300346	100.00%	10.919%
2	2.798	104	106	120	rBV3	4424	28140	1.22%	0.134%
3	4.719	272	274	292	rBV	204674	376019	16.35%	1.785%
4	5.187	314	315	338	rBV	789437	1550656	67.41%	7.360%
5	5.587	348	350	359	rVB	23745	28561	1.24%	0.136%
6	6.273	408	410	416	rBV	1006037	1566256	68.09%	7.434%
7	6.364	416	418	431	rVB	1159476	1663204	72.30%	7.894%
8	6.593	436	438	445	rBV	430041	456832	19.86%	2.168%
9	6.753	449	452	454	rBV	845398	1248308	54.27%	5.925%
10	7.165	486	488	499	rVB	814422	941257	40.92%	4.468%
11	7.885	548	551	562	rVB	477190	629064	27.35%	2.986%
12	8.959	642	645	648	rBV	2024285	1893497	82.31%	8.987%
13	9.256	667	671	672	rBV	30399	39853	1.73%	0.189%
14	9.359	678	680	683	rBV	503358	468607	20.37%	2.224%
15	9.496	690	692	694	rBV	23155	25225	1.10%	0.120%
16	9.622	701	703	706	rBV	525702	654628	28.46%	3.107%
17	10.422	770	773	775	rBV2	686431	994554	43.23%	4.721%
18	10.536	781	783	788	rVB	34646	50178	2.18%	0.238%
19	10.982	820	822	823	rBV	36983	31592	1.37%	0.150%
20	11.108	831	833	834	rBV	519392	611787	26.60%	2.904%
21	11.131	834	835	837	rVV	72508	63355	2.75%	0.301%
22	11.188	837	840	842	rVB	28731	45182	1.96%	0.214%
23	11.405	857	859	862	rVB	32233	32148	1.40%	0.153%
24	11.611	871	877	878	rBV4	24670	40995	1.78%	0.195%
25	11.634	878	879	882	rVV2	26309	59383	2.58%	0.282%
26	11.714	885	886	891	rVB	37472	54109	2.35%	0.257%
27	12.148	923	924	926	rBV	23444	33591	1.46%	0.159%
28	12.182	926	927	931	rVV3	16340	29217	1.27%	0.139%
29	12.251	931	933	936	rVB3	13447	24934	1.08%	0.118%
30	12.308	936	938	940	rBV	165405	160788	6.99%	0.763%
31	12.491	950	954	955	rBV3	15576	32525	1.41%	0.154%
32	12.536	955	958	962	rVV	167354	192658	8.38%	0.914%
33	12.685	968	971	973	rBV	1481430	1471069	63.95%	6.982%
34	12.754	975	977	980	rBV	17990	30761	1.34%	0.146%

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Stop Thrs : 0 Peak Location: TOP

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35	12.868	983	987	989	rBV	47886	70680	3.07%	0.335%
36	12.937	989	993	994	rBV2	34509	59320	2.58%	0.282%
37	12.971	994	996	1000	rVB	29352	46069	2.00%	0.219%
38	13.097	1005	1007	1011	rVV2	16008	29264	1.27%	0.139%
39	13.382	1030	1032	1034	rVB	26147	30504	1.33%	0.145%
40	13.485	1039	1041	1044	rVV3	24278	48337	2.10%	0.229%
41	13.588	1048	1050	1054	rVB2	83002	136533	5.94%	0.648%
42	13.725	1059	1062	1068	rBV2	515093	834190	36.26%	3.959%
43	13.828	1069	1071	1075	rBV3	16156	31415	1.37%	0.149%
44	13.897	1075	1077	1080	rBV3	18297	42750	1.86%	0.203%
45	14.125	1094	1097	1098	rBV	28445	47927	2.08%	0.227%
46	14.228	1102	1106	1111	rVB3	39132	131160	5.70%	0.623%
47	14.628	1139	1141	1144	rVV2	70834	74188	3.23%	0.352%
48	14.731	1147	1150	1154	rVV	129508	304672	13.24%	1.446%
49	14.788	1154	1155	1156	rVV	68623	57008	2.48%	0.271%
50	14.822	1156	1158	1163	rVB2	77762	119252	5.18%	0.566%
51	14.982	1170	1172	1174	rBV	87832	106803	4.64%	0.507%
52	15.040	1175	1177	1179	rVV	99607	129301	5.62%	0.614%
53	15.085	1179	1181	1188	rVB	364902	490254	21.31%	2.327%
54	15.462	1212	1214	1217	rBV	52133	92139	4.01%	0.437%
55	15.645	1228	1230	1236	rVB4	36700	86979	3.78%	0.413%
56	16.000	1258	1261	1266	rVB3	40958	82915	3.60%	0.394%
57	16.354	1290	1292	1295	rVB	45197	74994	3.26%	0.356%
58	16.731	1323	1325	1327	rBV	31395	61334	2.67%	0.291%
59	17.600	1398	1401	1405	rVB5	20661	50890	2.21%	0.242%

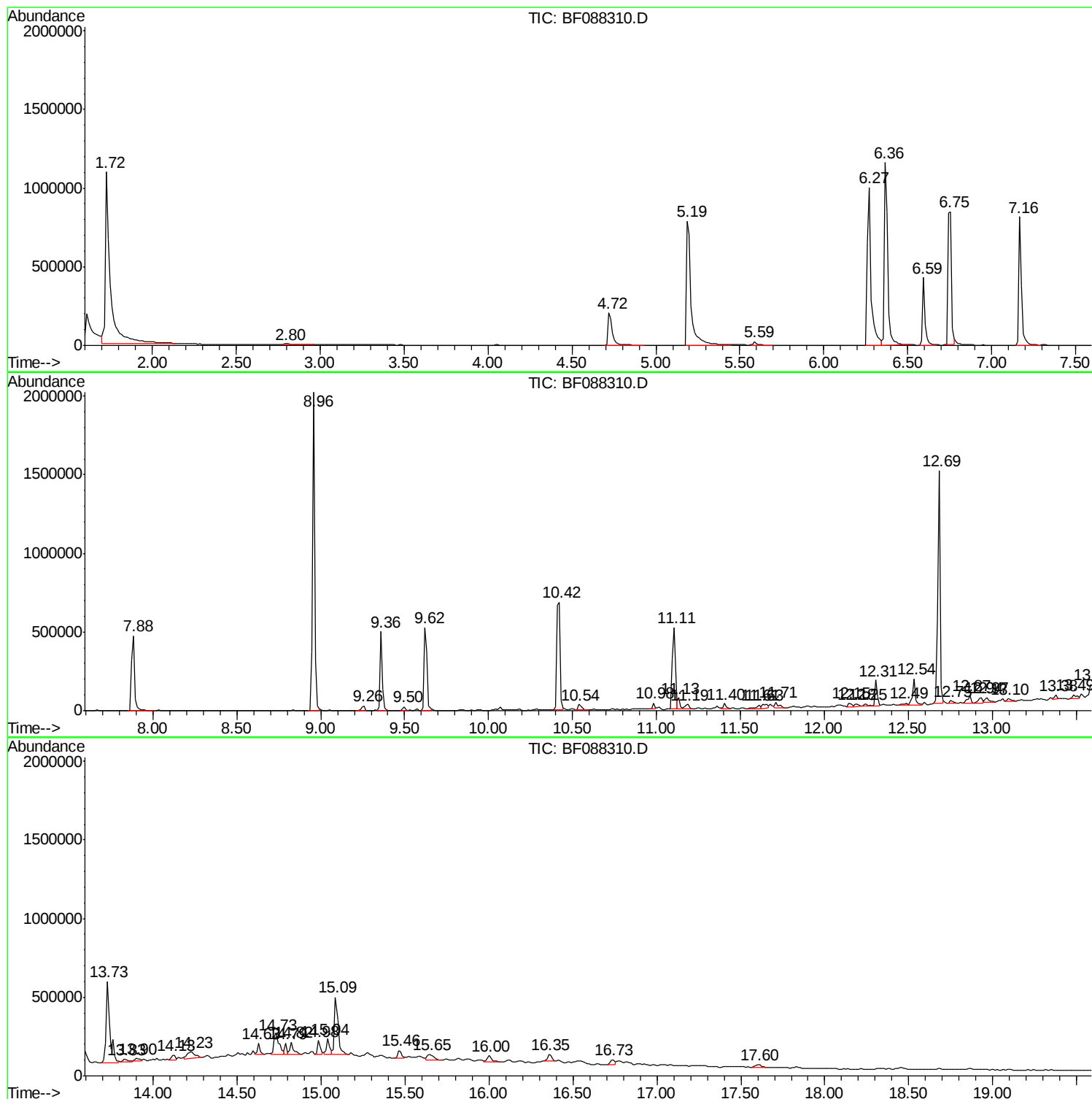
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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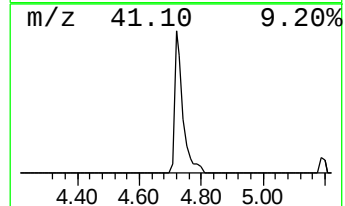
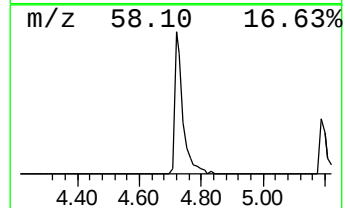
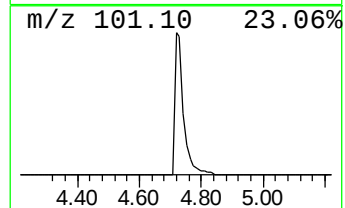
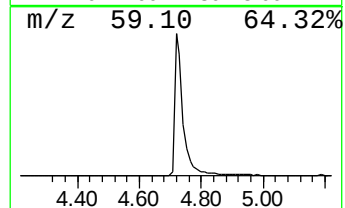
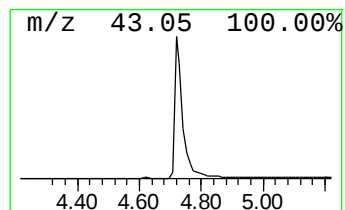
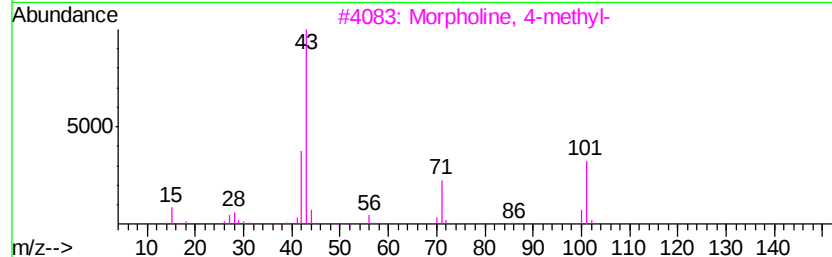
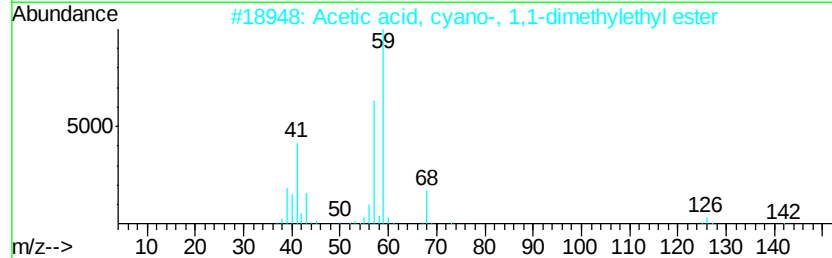
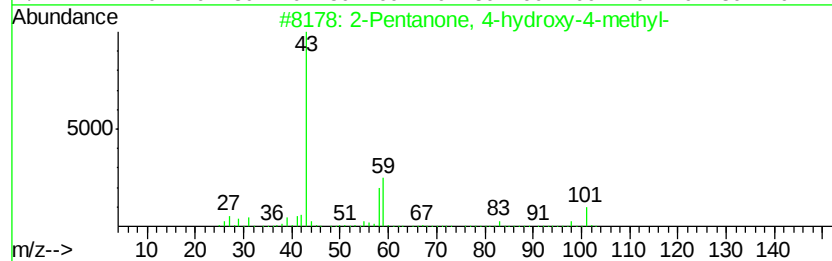
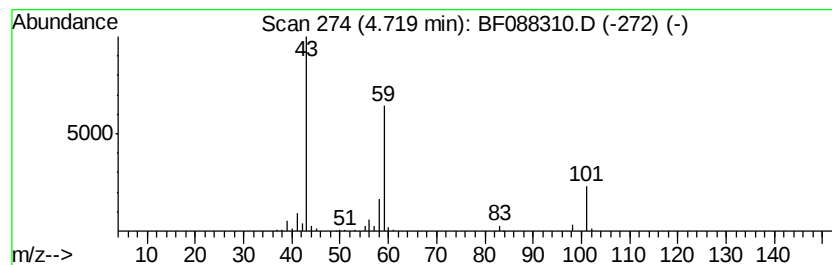
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.72	16.46 ng	376019	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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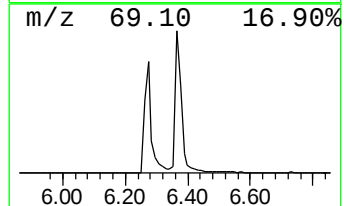
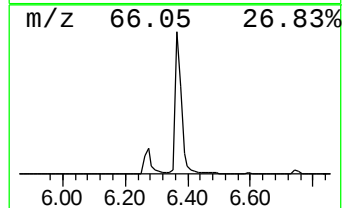
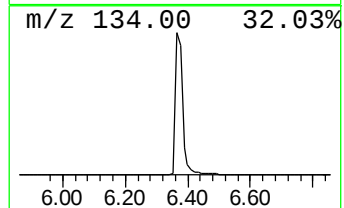
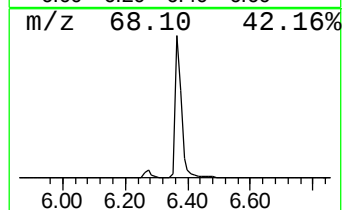
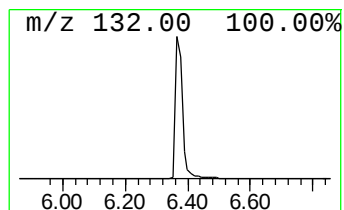
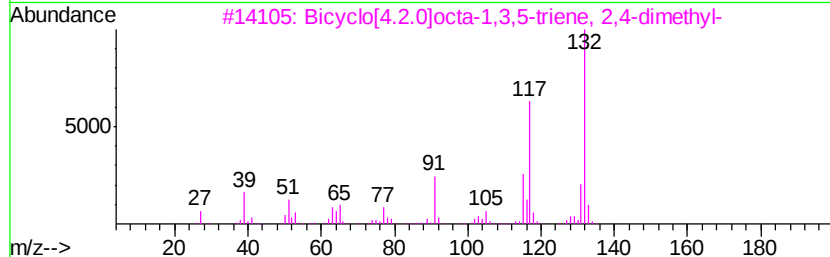
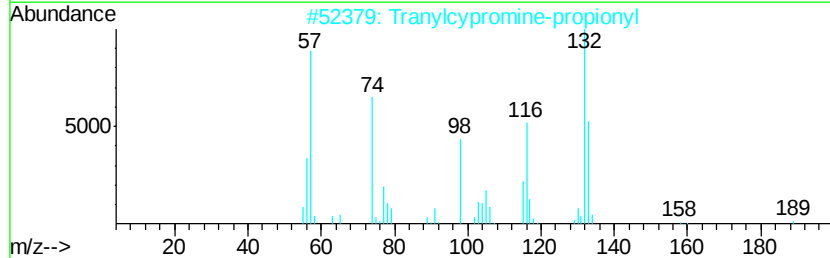
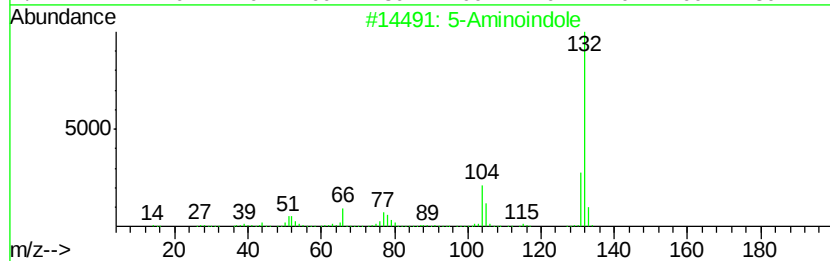
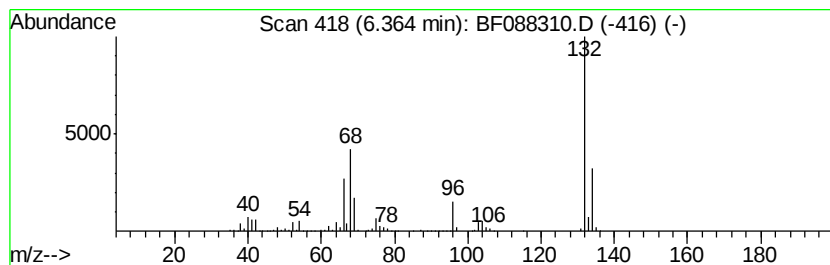
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TIC Library : C:\Database\NIST11.L
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Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	72.81 ng	1663200	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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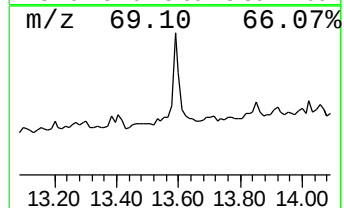
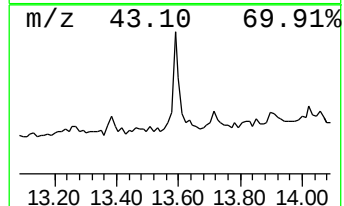
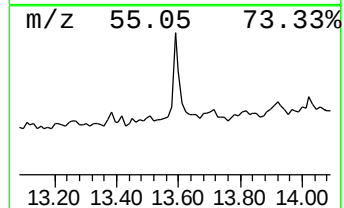
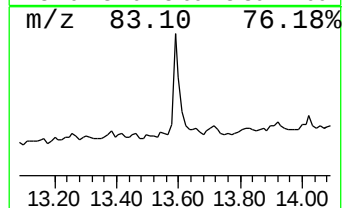
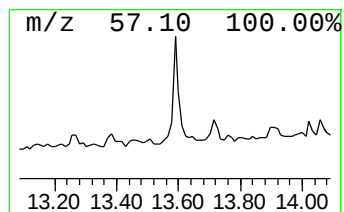
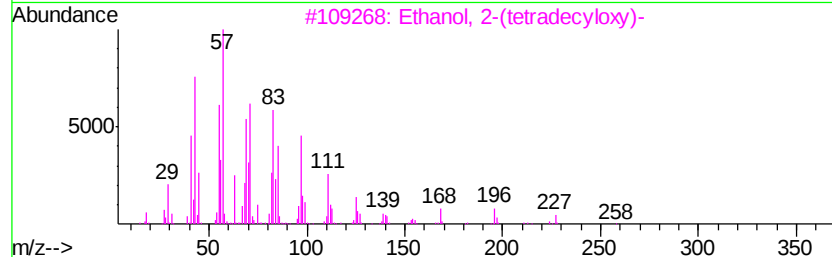
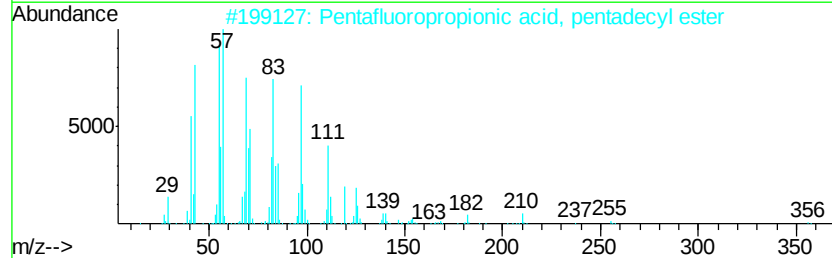
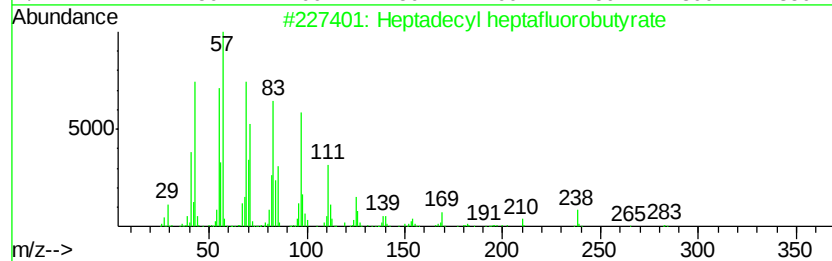
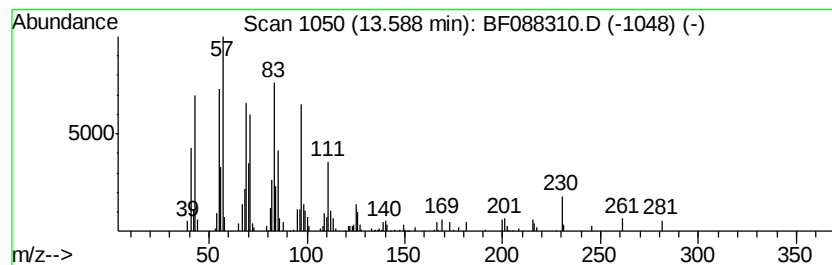
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	3.27 ng	136533	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	76
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76



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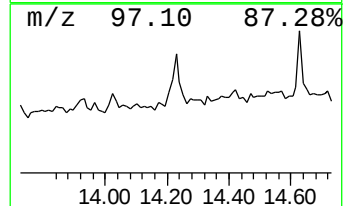
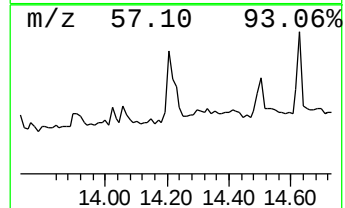
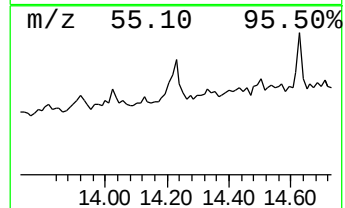
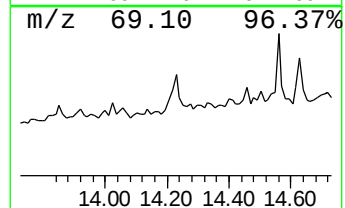
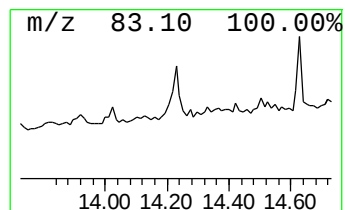
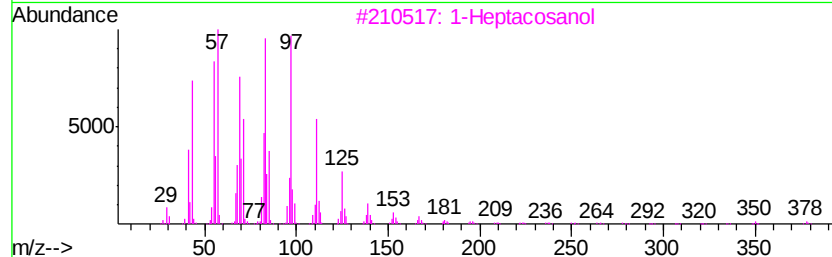
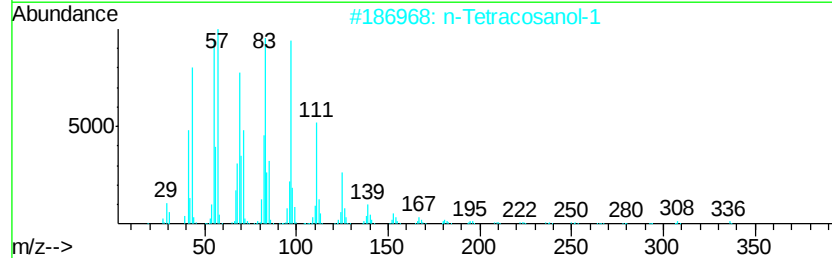
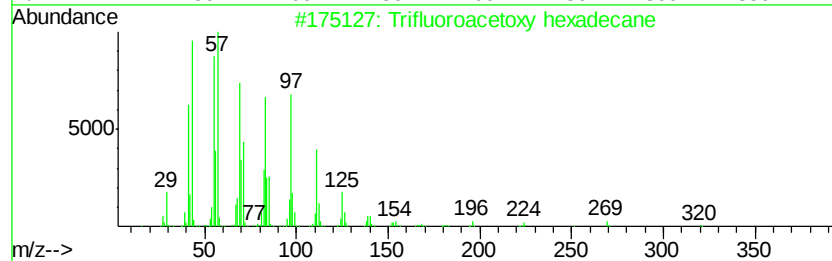
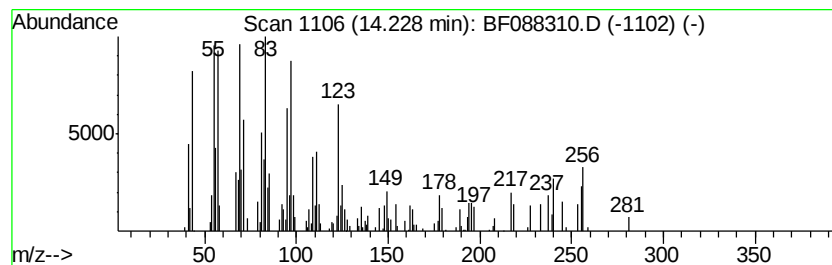
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.23	3.14 ng	131160	Chrysene-d12	13.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	86
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	84
3	1-Heptacosanol	396	C27H56O	002004-39-9	83
4	Behenic alcohol	326	C22H46O	000661-19-8	83
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	58



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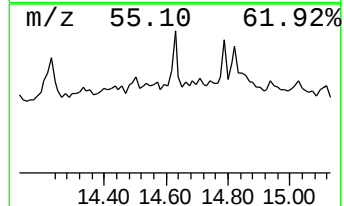
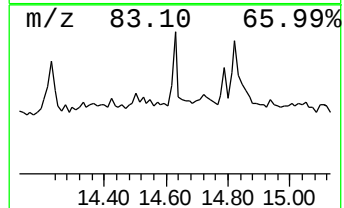
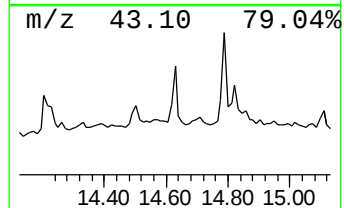
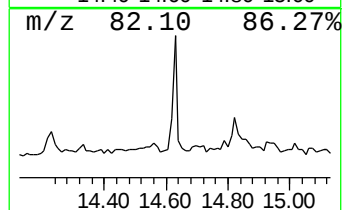
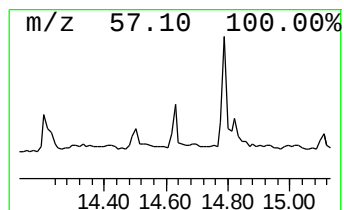
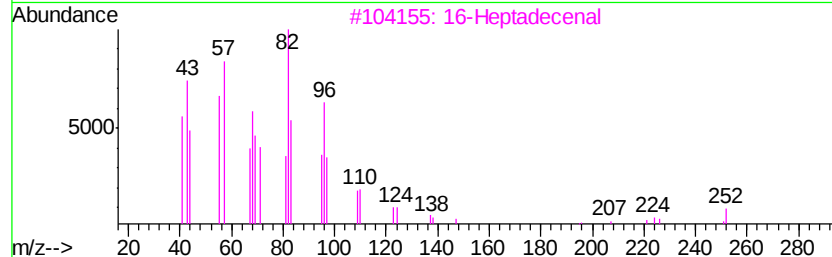
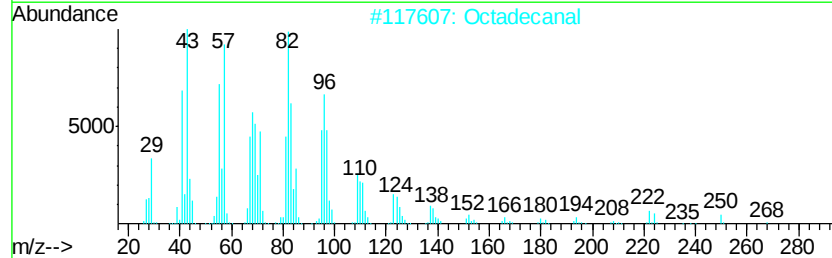
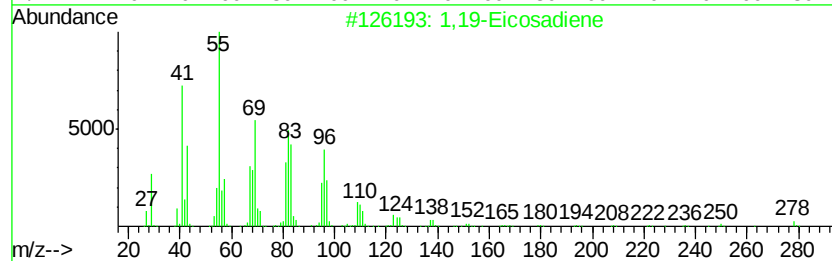
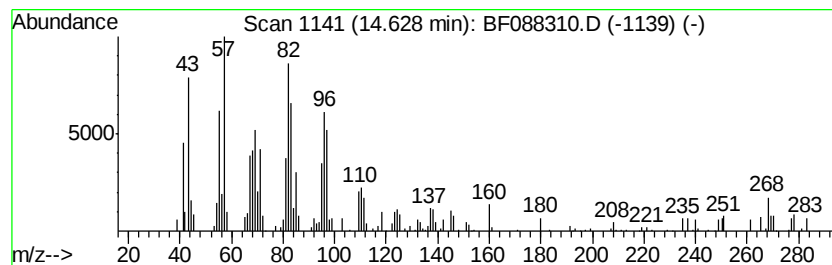
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ClientSampleId :
SB-3(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,19-Eicosadiene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.63	3.03 ng	74188	Perylene-d12	15.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	92
2	Octadecanal	268	C18H36O	000638-66-4	90
3	16-Heptadecenal	252	C17H32O	1000144-57-9	80
4	10-Octadecenal	266	C18H34O	056554-92-8	80
5	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088310.D
Acq On : 24 Jun 2016 1:34
Operator : UM/SJ
Sample : H3682-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

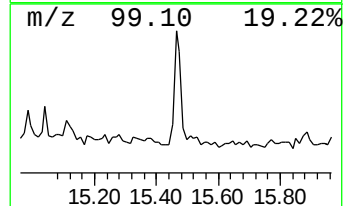
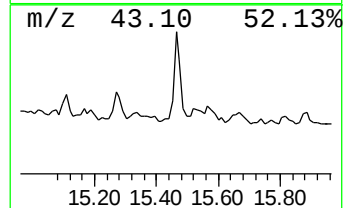
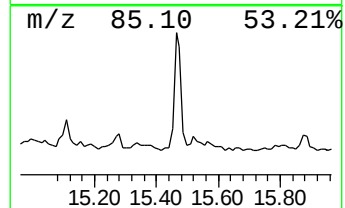
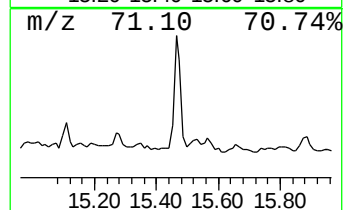
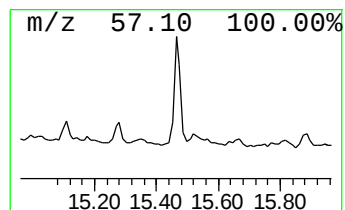
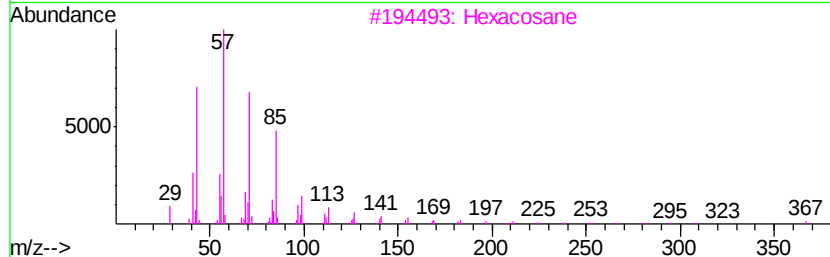
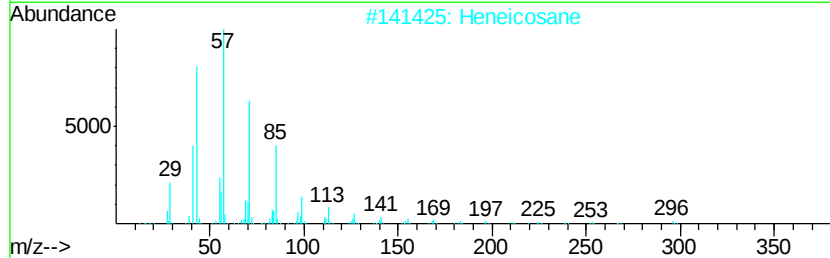
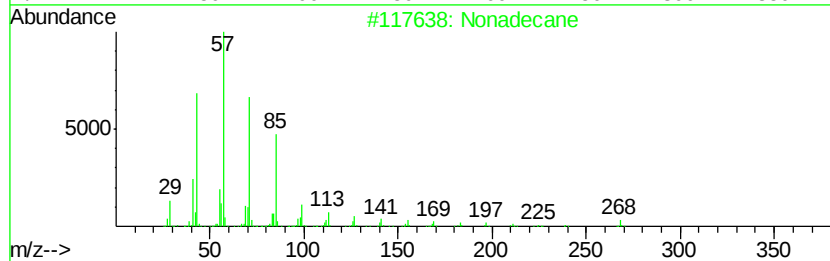
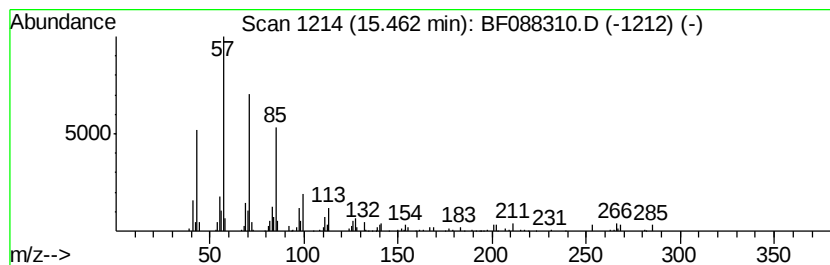
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.46	3.76 ng	92139	Perylene-d12	15.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Heneicosane	296	C21H44	000629-94-7	87
3	Hexacosane	366	C26H54	000630-01-3	83
4	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
5	Heptacosane	380	C27H56	000593-49-7	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088310.D
Acq On : 24 Jun 2016 1:34
Operator : UM/SJ
Sample : H3682-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(0-6)

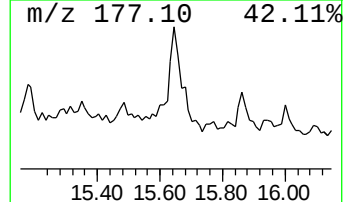
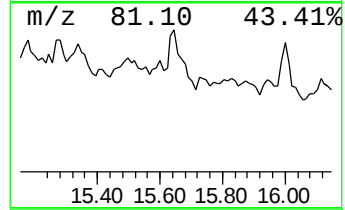
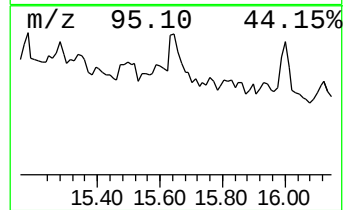
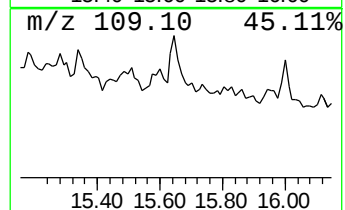
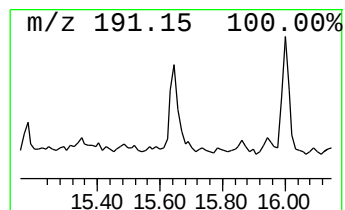
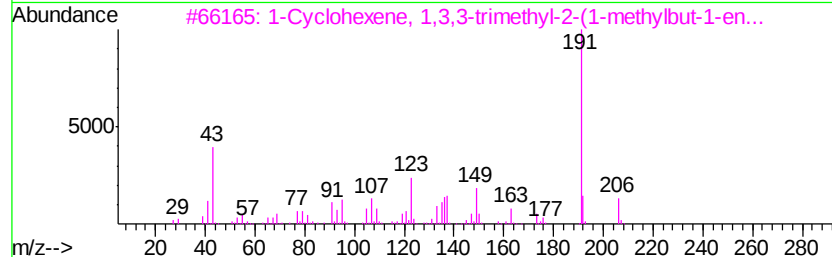
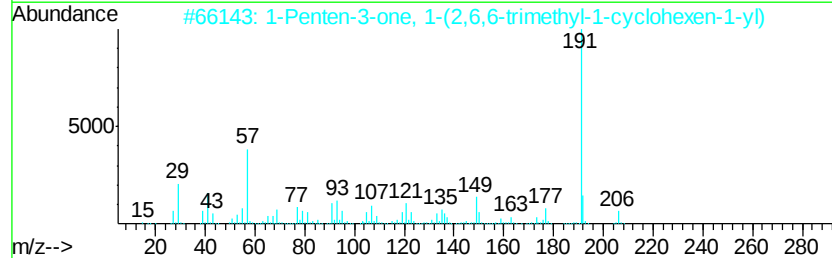
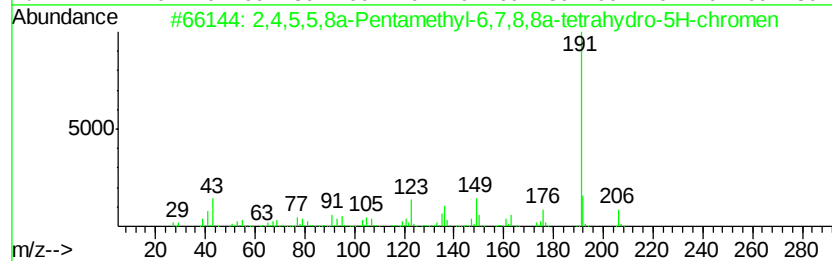
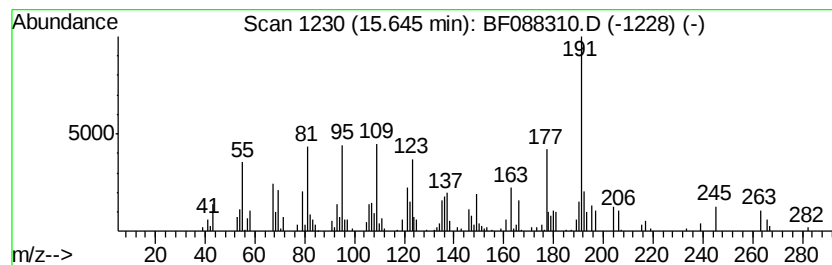
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2,4,5,5,8a-Pentamethyl-6,7,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	3.55 ng	86979	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	50		
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43		
3	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	41		
4	Amiphenazole	191	C9H9N3S	000490-55-1	35		
5	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	27		



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
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Acq On : 24 Jun 2016 1:34
Operator : UM/SJ
Sample : H3682-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

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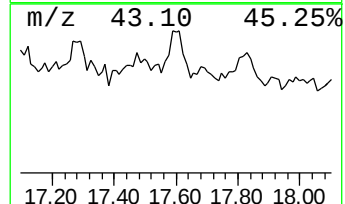
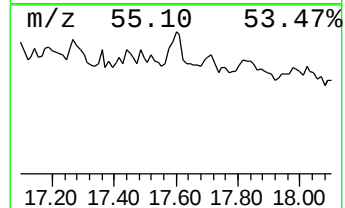
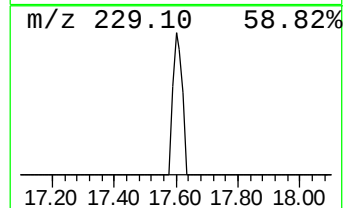
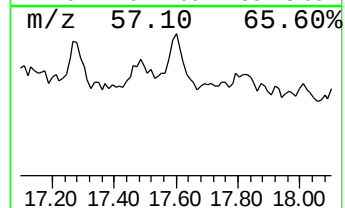
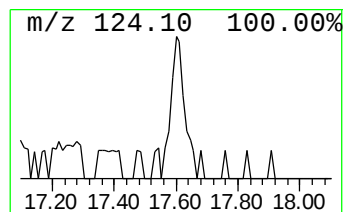
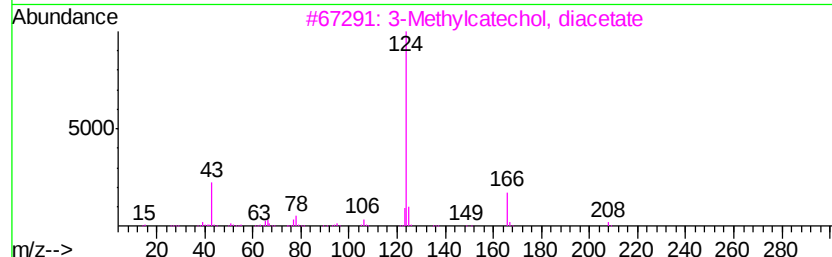
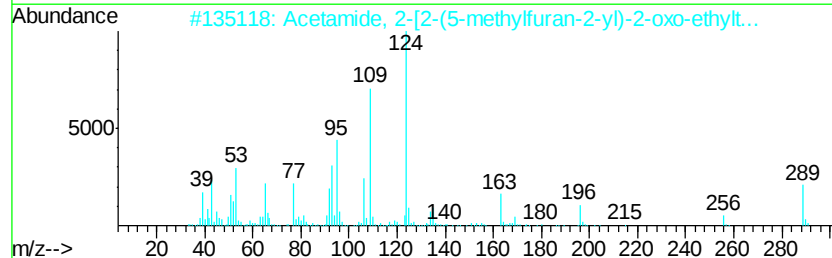
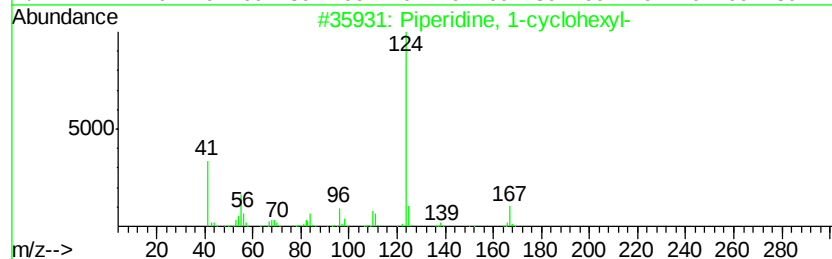
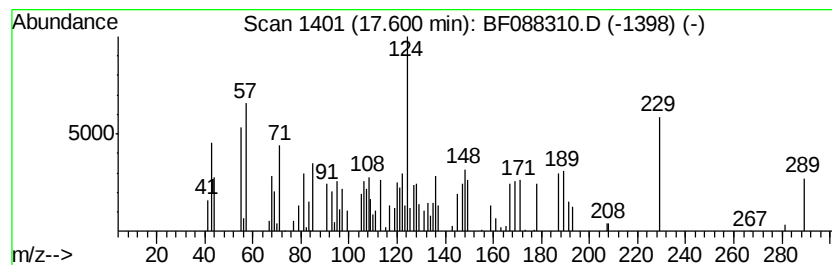
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.60 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	2.08 ng	50890	Perylene-d12	15.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Piperidine, 1-cyclohexyl-	167	C11H21N	003319-01-5	22
2		Acetamide, 2-[2-(5-methylfuran-2-yl)-2-oxo-ethyl]-	289	C15H15N03S	1000259-79-3	22
3		3-Methylcatechol, diacetate	208	C11H12O4	1000352-78-9	14
4		2-Methylresorcinol, diacetate	208	C11H12O4	1000352-78-4	14
5		N-(3-Amino-2-hydroxy-phenyl)-ace...	166	C8H10N2O2	1000186-23-1	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
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Acq On : 24 Jun 2016 1:34
Operator : UM/SJ
Sample : H3682-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.72	16.5	ng	376019	1	6.59	456832	20.0
unknown6.36	6.36	72.8	ng	1663200	1	6.59	456832	20.0
Heptadecyl heptaf...	13.59	3.3	ng	136533	5	13.73	834190	20.0
Trifluoroacetoxy ...	14.23	3.1	ng	131160	5	13.73	834190	20.0
1,19-Eicosadiene	14.63	3.0	ng	74188	6	15.09	490254	20.0
Nonadecane	15.46	3.8	ng	92139	6	15.09	490254	20.0
2,4,5,5,8a-Pentam...	15.65	3.5	ng	86979	6	15.09	490254	20.0
unknown17.60	17.60	2.1	ng	50890	6	15.09	490254	20.0