

Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
 Data File : BF093775.D
 Acq On : 20 Mar 2017 20:20
 Operator : SJ/MA
 Sample : I2304-01 2X
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-A(0-5)B1

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-BF032017.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.104	16	19	21	rVB2	49197	71343	2.40%	0.211%
2	5.007	270	273	278	rBV	370624	510470	17.16%	1.508%
3	5.430	307	310	312	rBV	2913172	2707676	91.01%	8.001%
4	5.841	343	346	348	rBV	33512	33097	1.11%	0.098%
5	6.459	397	400	403	rBV	2428296	2816042	94.65%	8.321%
6	6.596	410	412	415	rBV	2528472	2840602	95.48%	8.394%
7	6.836	431	433	435	rBV	1759536	1466234	49.28%	4.332%
8	6.996	444	447	449	rBV	2196142	2272678	76.39%	6.715%
9	7.396	479	482	484	rBV	2080958	2001181	67.26%	5.913%
10	7.453	484	487	488	rVB	31260	30680	1.03%	0.091%
11	7.636	499	503	507	rBV3	33408	69995	2.35%	0.207%
12	7.853	518	522	524	rBV4	26373	46412	1.56%	0.137%
13	8.116	543	545	548	rBV	1671810	1861027	62.55%	5.499%
14	8.230	553	555	558	rVB	28525	37638	1.27%	0.111%
15	8.424	566	572	576	rBV6	19261	53958	1.81%	0.159%
16	8.562	582	584	586	rBV	49674	58864	1.98%	0.174%
17	8.722	596	598	602	rBV2	56656	100081	3.36%	0.296%
18	8.825	605	607	609	rVB	30159	42578	1.43%	0.126%
19	8.927	614	616	622	rVB2	25107	41745	1.40%	0.123%
20	9.156	635	636	637	rBV	66584	54801	1.84%	0.162%
21	9.202	637	640	642	rVB	2505290	2975073	100.00%	8.791%
22	9.293	645	648	650	rBV	150877	157460	5.29%	0.465%
23	9.453	660	662	666	rBV2	41529	71717	2.41%	0.212%
24	9.533	666	669	672	rBV2	63009	152751	5.13%	0.451%
25	9.590	672	674	675	rVV	327609	305138	10.26%	0.902%
26	9.636	677	678	682	rVB4	28372	64208	2.16%	0.190%
27	9.819	693	694	696	rVB	217050	161733	5.44%	0.478%
28	9.876	696	699	701	rBV	1704977	2058301	69.18%	6.082%
29	9.979	705	708	711	rVB3	29638	52926	1.78%	0.156%
30	10.082	712	717	718	rBV4	47375	109518	3.68%	0.324%
31	10.116	718	720	721	rVB2	28530	37917	1.27%	0.112%
32	10.139	721	722	724	rVB2	59414	65672	2.21%	0.194%
33	10.185	724	726	728	rBV2	27978	55942	1.88%	0.165%
34	10.288	730	735	736	rBV5	41311	107077	3.60%	0.316%

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35	10.322	736	738	739	rVB	145000	169301	5.69%	0.500%
36	10.368	739	742	745	rVB4	21233	42556	1.43%	0.126%
37	10.436	745	748	750	rBV3	27811	57483	1.93%	0.170%
38	10.539	754	757	760	rBV	144090	164619	5.53%	0.486%
39	10.585	760	761	763	rVB	35107	30290	1.02%	0.090%
40	10.619	763	764	765	rBV	42771	45963	1.54%	0.136%
41	10.653	765	767	769	rVB	1366990	1283099	43.13%	3.791%
42	10.699	769	771	774	rBV4	15498	34132	1.15%	0.101%
43	10.790	777	779	783	rBV	266553	452374	15.21%	1.337%
44	10.985	795	796	798	rBV2	34097	42705	1.44%	0.126%
45	11.110	805	807	809	rVB3	28205	44597	1.50%	0.132%
46	11.236	816	818	819	rBV	222814	189496	6.37%	0.560%
47	11.270	819	821	823	rVB	164272	170253	5.72%	0.503%
48	11.350	826	828	829	rBV	1843198	1746529	58.71%	5.161%
49	11.613	849	851	853	rBV	49926	56573	1.90%	0.167%
50	11.659	853	855	858	rVV	189045	158006	5.31%	0.467%
51	11.842	867	871	873	rBV5	47554	144408	4.85%	0.427%
52	11.956	880	881	887	rVB5	45261	110329	3.71%	0.326%
53	12.071	889	891	893	rVV	83762	102055	3.43%	0.302%
54	12.345	913	915	918	rBV	69159	91541	3.08%	0.270%
55	12.448	923	924	926	rVB	67964	92346	3.10%	0.273%
56	12.562	932	934	935	rBV2	60416	90112	3.03%	0.266%
57	12.825	956	957	960	rBV	84139	87390	2.94%	0.258%
58	12.928	964	966	969	rVV	2001347	1913961	64.33%	5.655%
59	13.179	986	988	989	rBV2	68573	57990	1.95%	0.171%
60	13.831	1043	1045	1051	rVB	215637	405380	13.63%	1.198%
61	13.968	1055	1057	1059	rBV	1000734	1094286	36.78%	3.233%
62	15.385	1178	1181	1183	rVB	712410	1030503	34.64%	3.045%
63	16.060	1238	1240	1249	rVB4	87356	246692	8.29%	0.729%
64	16.471	1273	1276	1279	rVB	107801	195263	6.56%	0.577%

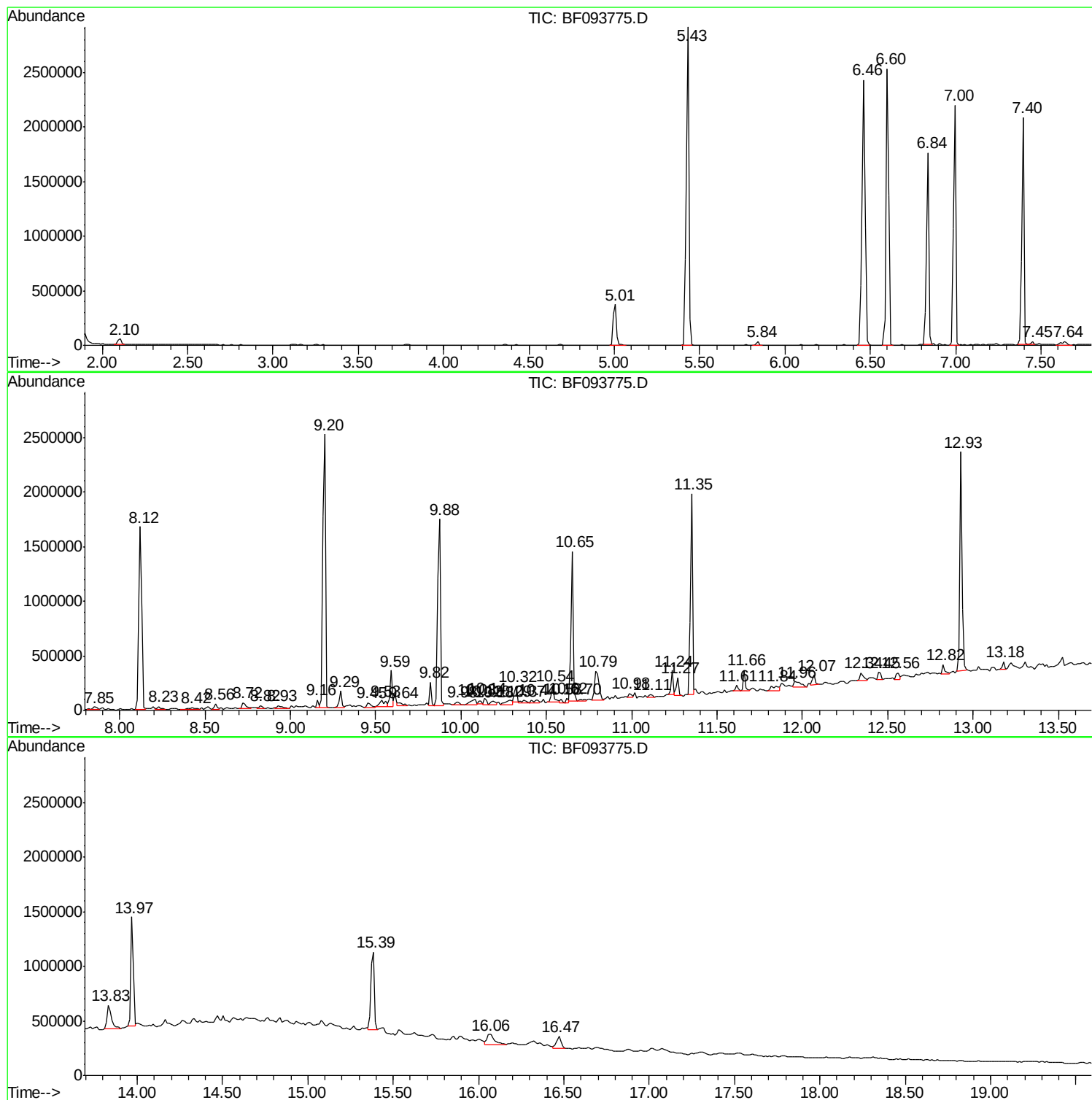
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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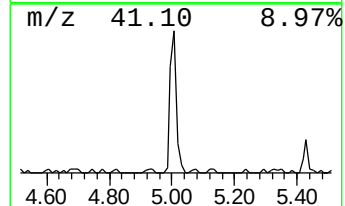
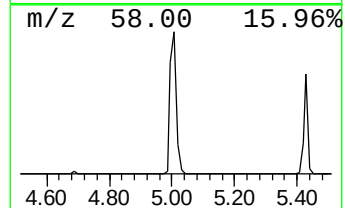
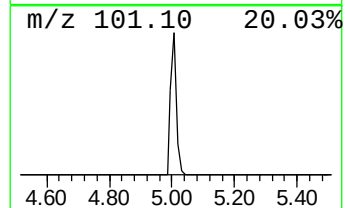
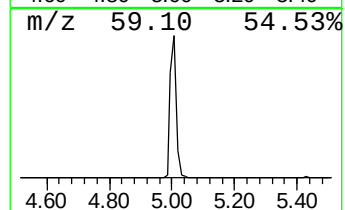
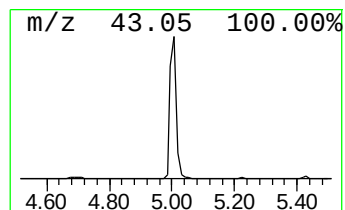
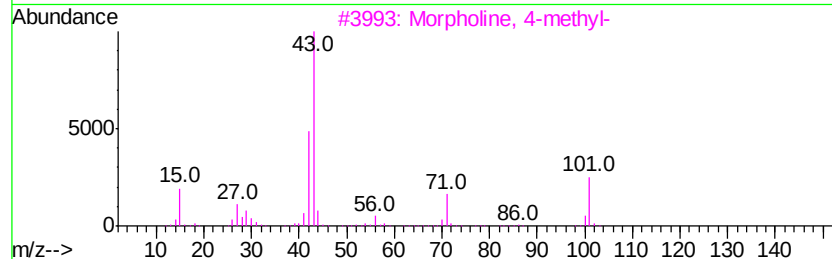
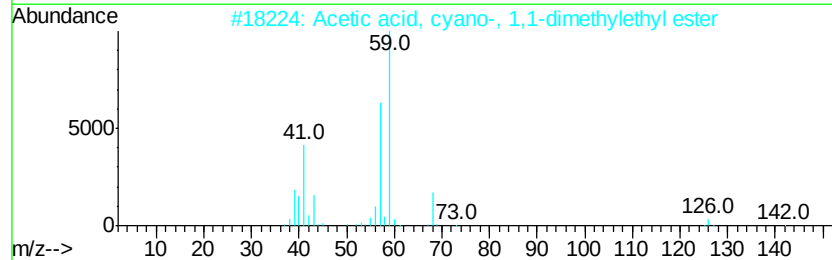
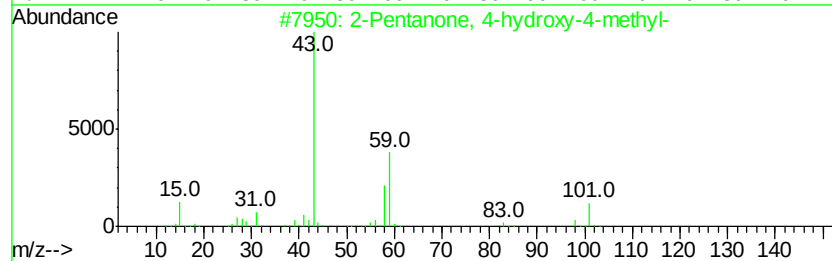
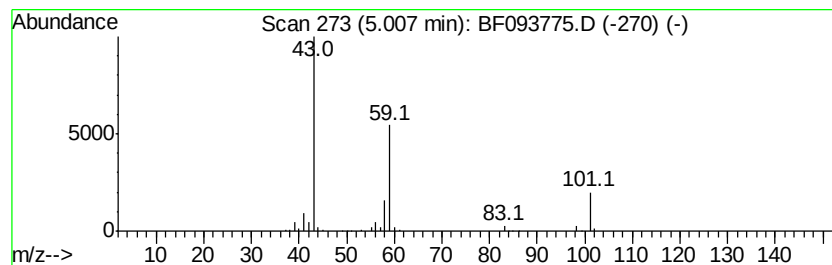
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	6.96 ng	510470	1,4-Dichlorobenzene-d4	6.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5			4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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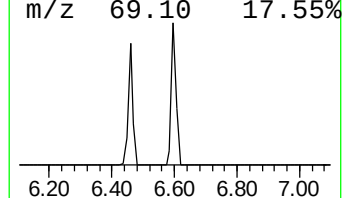
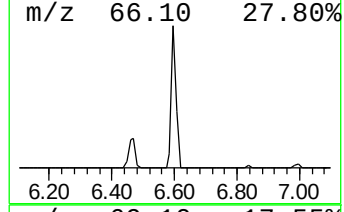
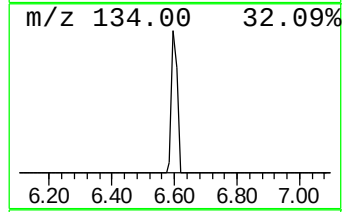
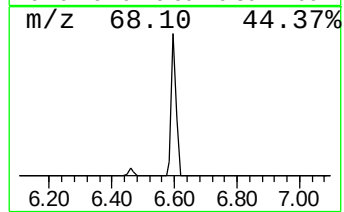
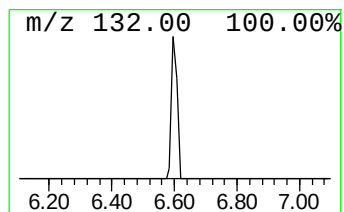
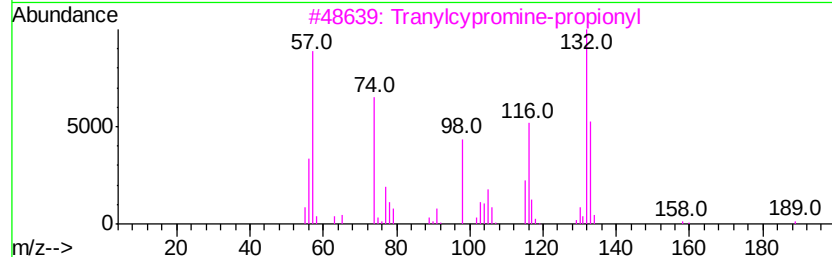
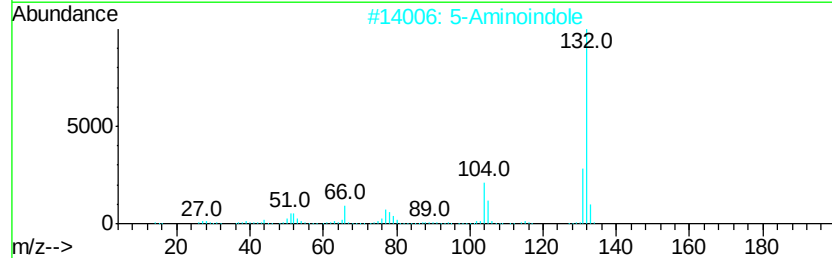
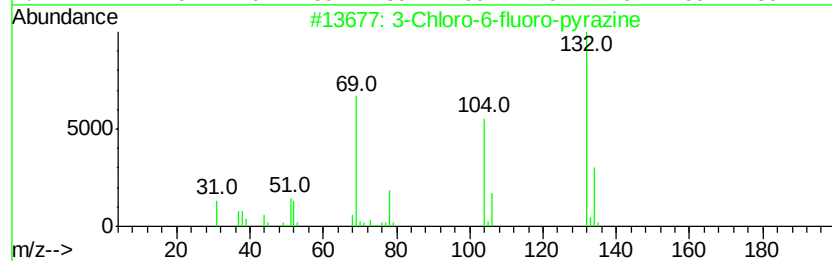
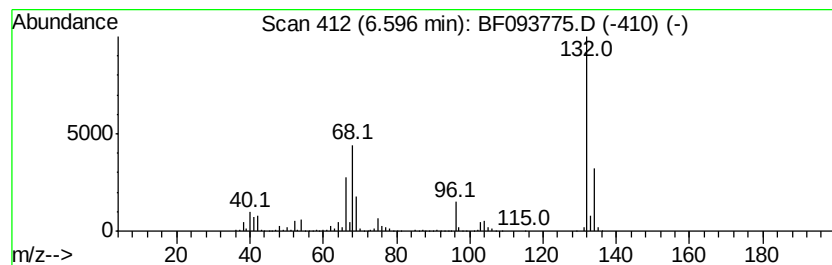
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	38.75 ng	2840600	1,4-Dichlorobenzene-d4	6.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole			132	C8H8N2	005192-03-0	12
3	Tranvlcypropine-propionyl			189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...			132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine			132	C4H2ClFN2	051422-00-5	9



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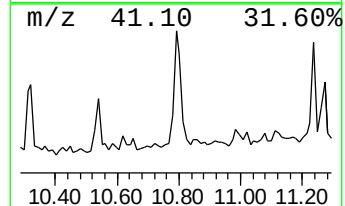
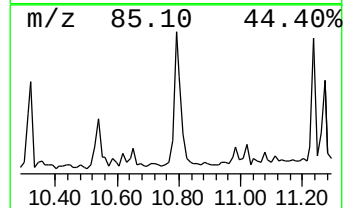
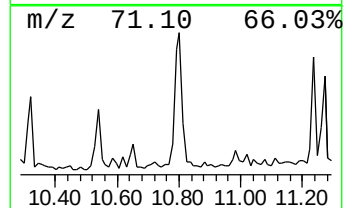
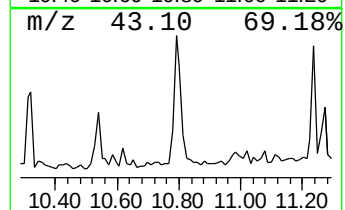
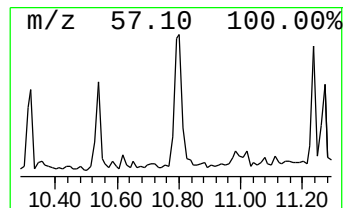
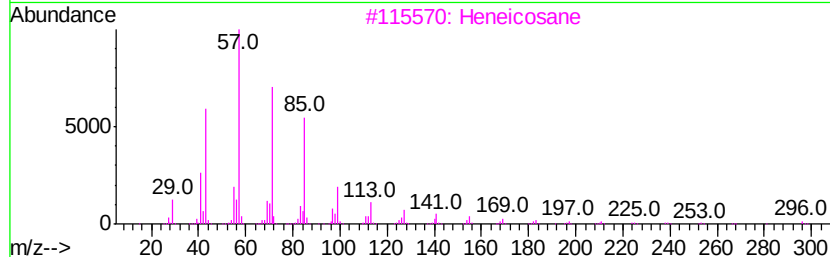
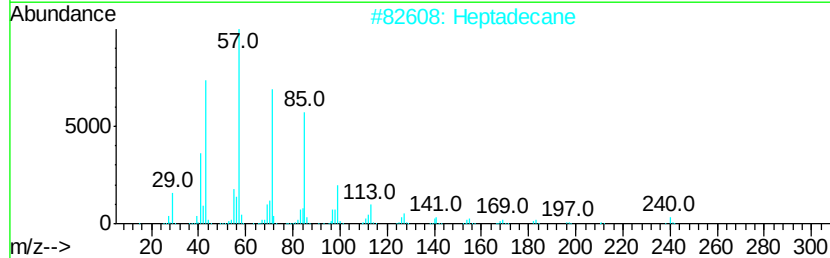
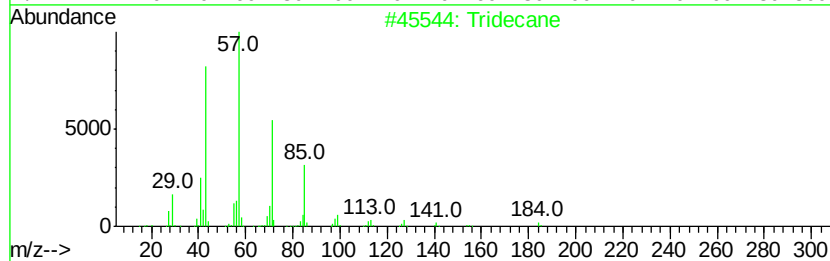
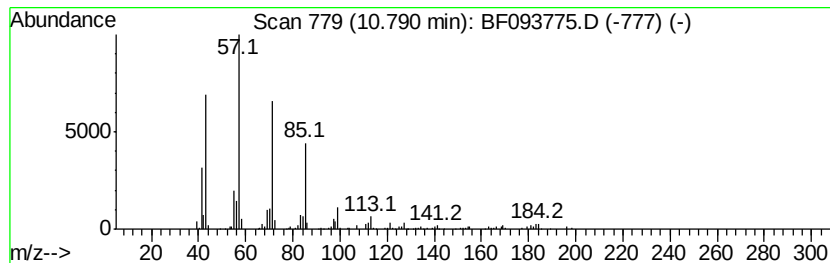
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Peak Number 4 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	5.18 ng	452374	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	93
2		Heptadecane	240	C17H36	000629-78-7	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Eicosane	282	C20H42	000112-95-8	87



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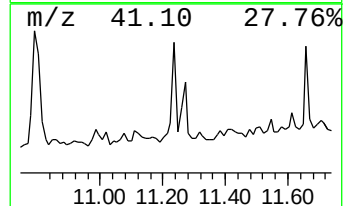
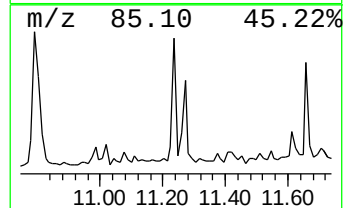
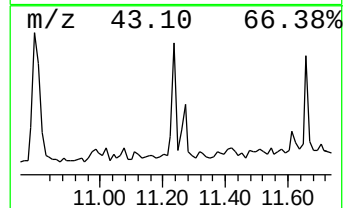
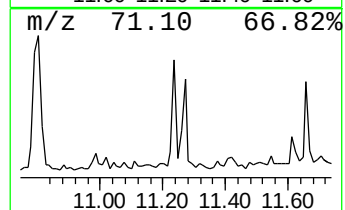
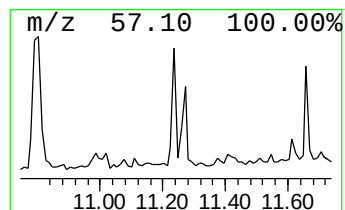
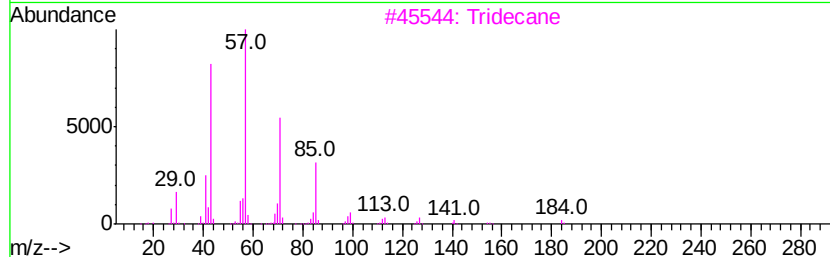
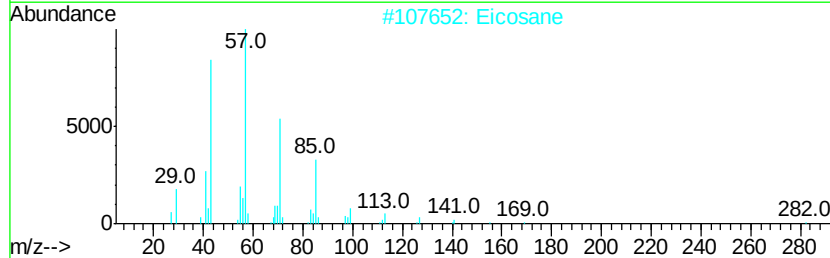
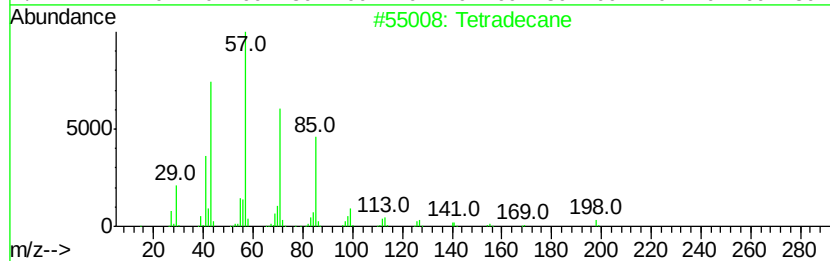
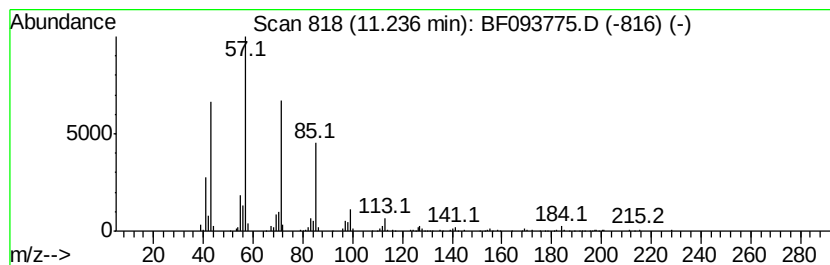
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.24	2.17 ng	189496	Phenanthrene-d10	11.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	91
2		Eicosane	282	C20H42	000112-95-8	83
3		Tridecane	184	C13H28	000629-50-5	81
4		Undecane, 2-methyl-	170	C12H26	007045-71-8	80
5		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80



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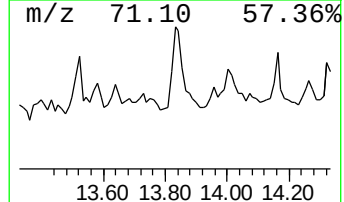
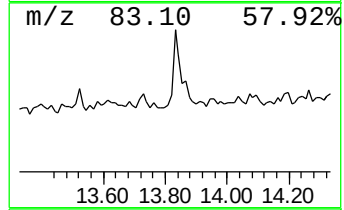
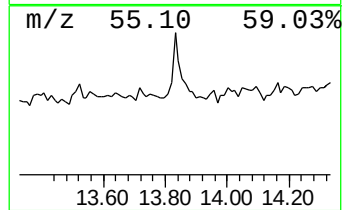
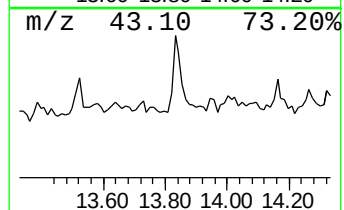
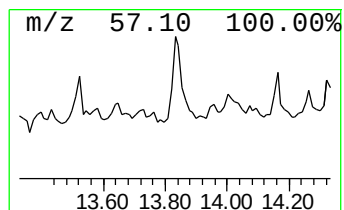
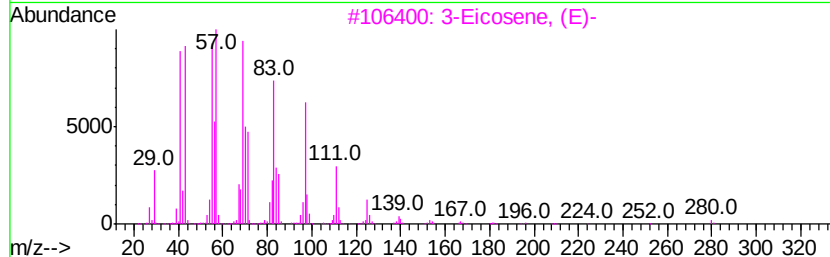
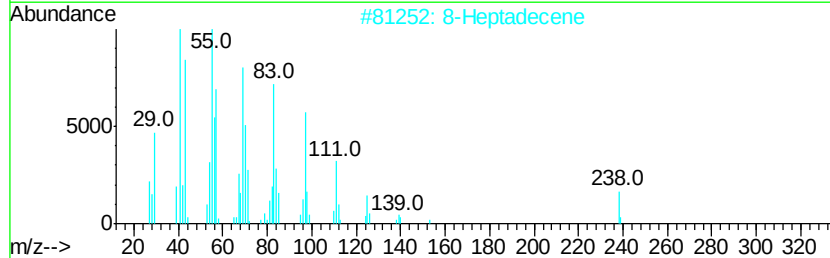
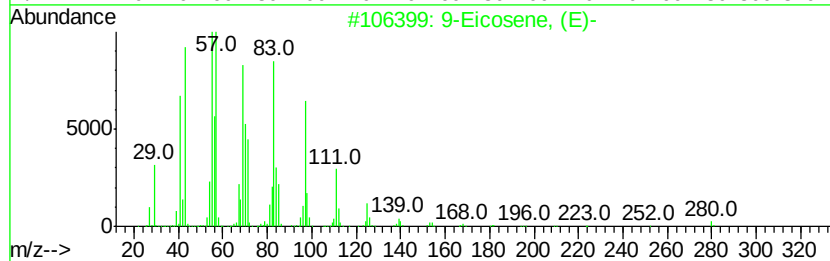
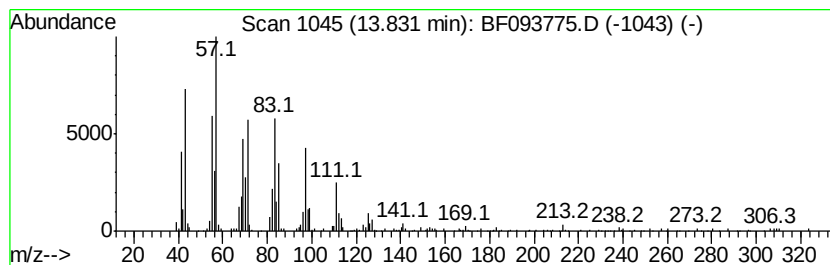
Instrument :
BNA_F
ClientSampleId :
SP-A(0-5)B1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.83	7.41 ng	405380	Chrysene-d12	13.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
2	8-Heptadecene	238	C17H34	054290-12-9	92
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
Data File : BF093775.D
Acq On : 20 Mar 2017 20:20
Operator : SJ/MA
Sample : I2304-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A(0-5)B1

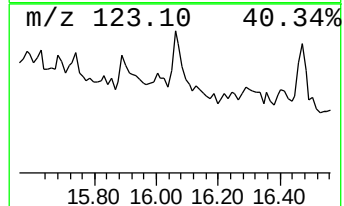
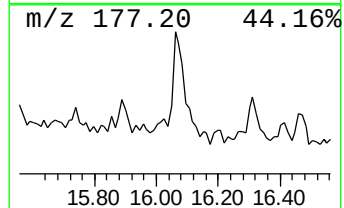
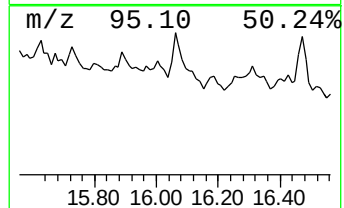
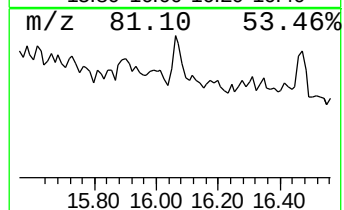
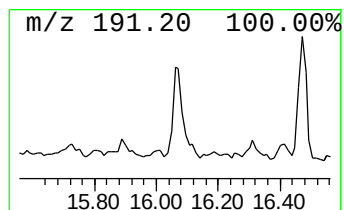
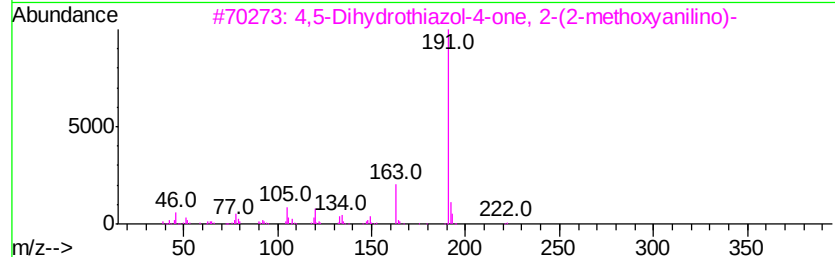
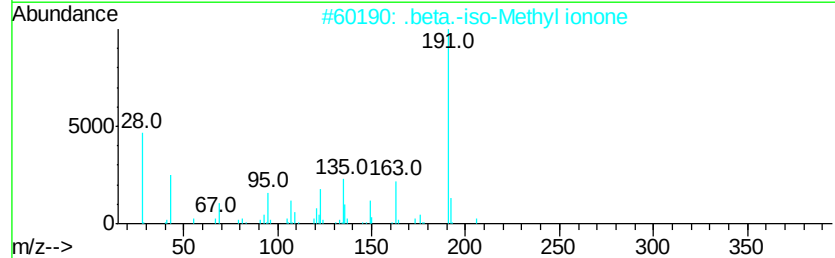
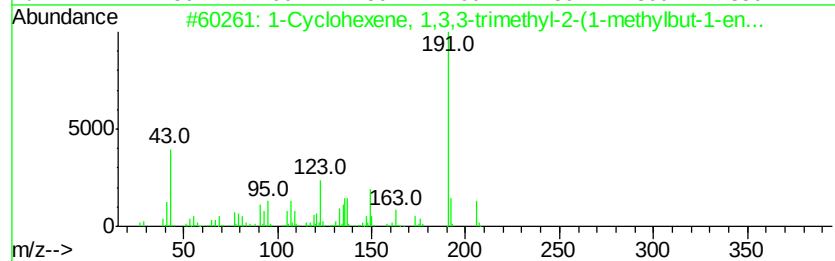
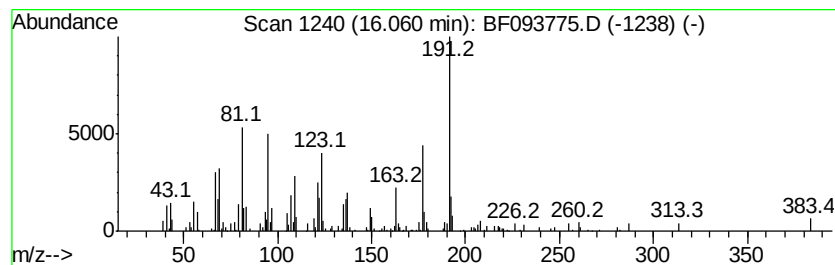
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.06 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	4.79 ng	246692	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
2		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	38
3		4,5-Dihydrothiazol-4-one, 2-(2-m...	222	C10H10N2O2S	022476-61-5	38
4		Propenamide, 3-(3,4-dimethoxyph...	313	C18H19N04	339165-72-9	32
5		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093775.D
Acq On : 20 Mar 2017 20:20
Operator : SJ/MA
Sample : I2304-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

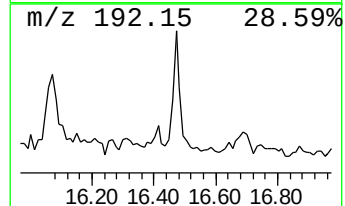
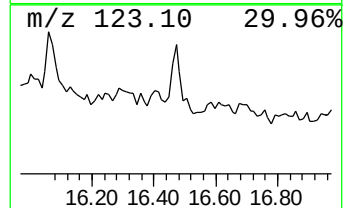
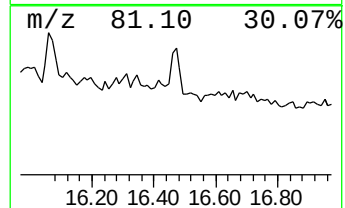
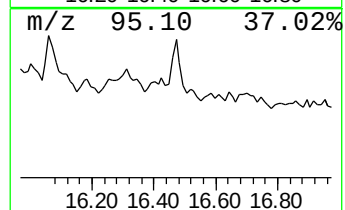
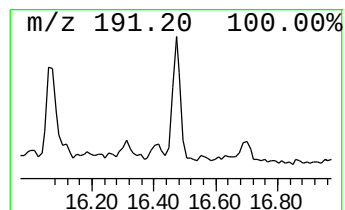
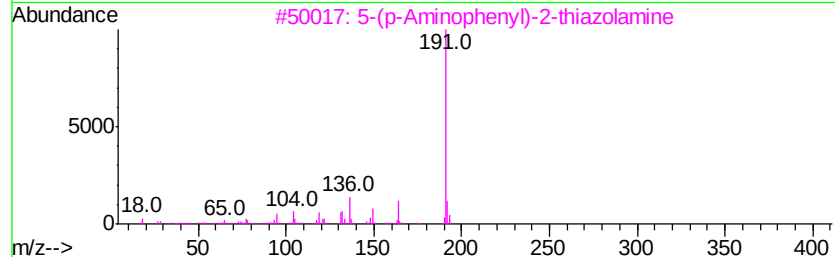
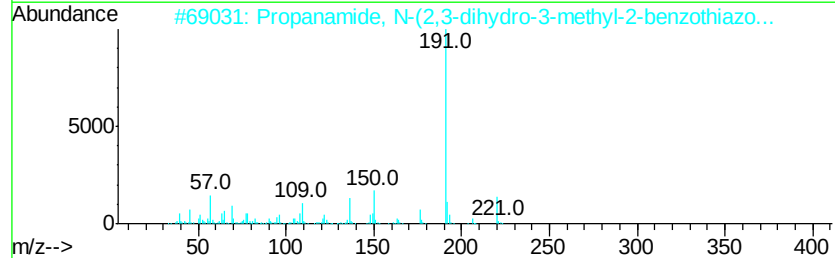
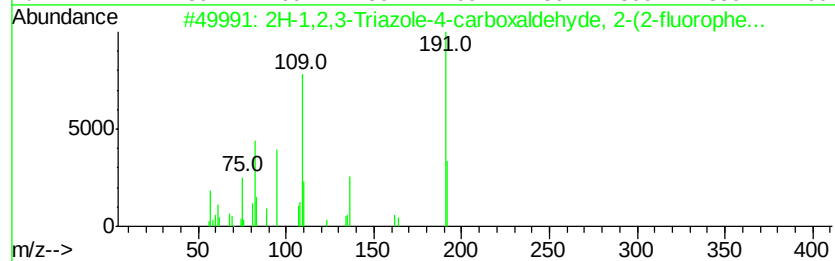
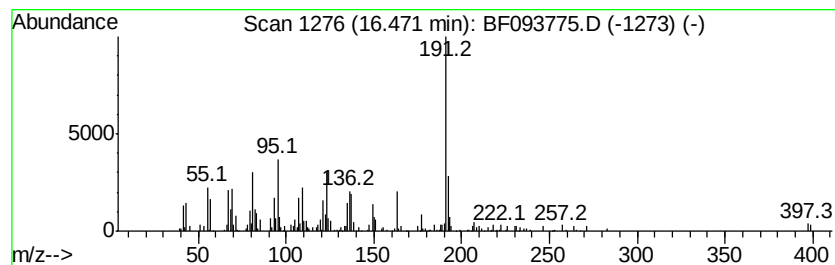
Instrument :
BNA_F
ClientSampleId :
SP-A(0-5)B1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2H-1,2,3-Triazole-4-carboxaldehyde... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.47	3.79 ng	195263	Perylene-d12		15.39		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-1,2,3-Triazole-4-carboxaldehv...	191	C9H6FN3O	051306-43-5	50
2			Propanamide, N-(2,3-dihydro-3-me...	220	C11H12N2OS	332413-15-7	47
3			5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	46
4			1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	40
5			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093775.D
Acq On : 20 Mar 2017 20:20
Operator : SJ/MA
Sample : I2304-01 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-A(0-5)B1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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-Pentanone, 4-hy...	5.01	7.0	ng	510470	1	6.84	1466230	20.0
unknown6.60	6.60	38.8	ng	2840600	1	6.84	1466230	20.0
Tridecane	10.79	5.2	ng	452374	4	11.35	1746530	20.0
Tetradecane	11.24	2.2	ng	189496	4	11.35	1746530	20.0
9-Eicosene, (E)-	13.83	7.4	ng	405380	5	13.97	1094290	20.0
unknown16.06	16.06	4.8	ng	246692	6	15.39	1030500	20.0
2H-1,2,3-Triazole...	16.47	3.8	ng	195263	6	15.39	1030500	20.0