

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
 Data File : BF084889.D
 Acq On : 6 Feb 2016 4:50
 Operator : SJ/IZ
 Sample : H1329-06
 Misc :
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-B006(21.5-23.5)

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-BF020116.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	4.807	236	238	250	rVB	828149	1415658	31.60%	3.111%
2	5.253	275	277	280	rBV	3639937	4480294	100.00%	9.844%
3	6.316	367	370	373	rBV	3960912	4273794	95.39%	9.391%
4	6.430	377	380	383	rBV	4511656	4336078	96.78%	9.527%
5	6.659	398	400	402	rBV	1320718	1065051	23.77%	2.340%
6	6.819	411	414	416	rBV	4142134	3724359	83.13%	8.183%
7	7.230	447	450	453	rBV	2649057	2777989	62.00%	6.104%
8	7.950	510	513	515	rBV	1429180	1387510	30.97%	3.049%
9	9.025	604	607	610	rBV	4330846	4256433	95.00%	9.352%
10	9.425	640	642	644	rBV	674749	537863	12.01%	1.182%
11	9.642	659	661	663	rBV	67532	55972	1.25%	0.123%
12	9.699	663	666	668	rBV	1363270	1397616	31.19%	3.071%
13	10.145	699	705	706	rBV	81770	92157	2.06%	0.202%
14	10.488	732	735	737	rBV	2841045	3056138	68.21%	6.715%
15	10.613	744	746	751	rVB	104799	121653	2.72%	0.267%
16	11.173	792	795	796	rBV	1532827	1313484	29.32%	2.886%
17	11.196	796	797	799	rVV	239733	179004	4.00%	0.393%
18	11.242	799	801	803	rVB2	52751	71467	1.60%	0.157%
19	11.413	813	816	820	rBV3	12913	44830	1.00%	0.099%
20	11.699	840	841	844	rVB2	52498	58780	1.31%	0.129%
21	11.779	847	848	853	rVB	57328	98607	2.20%	0.217%
22	11.893	853	858	862	rBV2	49935	91865	2.05%	0.202%
23	12.225	884	887	889	rBV	39882	70098	1.56%	0.154%
24	12.282	890	892	893	rVB	65363	63246	1.41%	0.139%
25	12.305	893	894	897	rVB	64555	58927	1.32%	0.129%
26	12.374	898	900	902	rBV	315815	418160	9.33%	0.919%
27	12.522	910	913	917	rBV2	25315	58349	1.30%	0.128%
28	12.602	917	920	922	rVV2	546312	634130	14.15%	1.393%
29	12.648	922	924	928	rVB3	78132	154419	3.45%	0.339%
30	12.762	932	934	936	rVB	3818731	3509204	78.33%	7.711%
31	12.934	946	949	951	rVB2	37218	70722	1.58%	0.155%
32	13.002	951	955	957	rBV2	94763	136006	3.04%	0.299%
33	13.036	957	958	962	rVB	73557	77291	1.73%	0.170%
34	13.242	973	976	979	rVB4	36528	57409	1.28%	0.126%

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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

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35	13.299	979	981	983	rBV	153703	158359	3.53%	0.348%
36	13.345	983	985	990	rVB	108222	123651	2.76%	0.272%
37	13.436	991	993	997	rVB	40068	70150	1.57%	0.154%
38	13.551	1000	1003	1004	rBV	49982	71037	1.59%	0.156%
39	13.677	1011	1014	1021	rVB2	332743	648845	14.48%	1.426%
40	13.802	1022	1025	1030	rVB2	1190276	1462590	32.64%	3.214%
41	13.997	1039	1042	1047	rVB2	84893	158471	3.54%	0.348%
42	14.191	1054	1059	1060	rBV	57181	86649	1.93%	0.190%
43	14.294	1066	1068	1075	rVB2	101681	161211	3.60%	0.354%
44	14.591	1091	1094	1096	rBV2	105873	129530	2.89%	0.285%
45	14.659	1097	1100	1104	rVV4	31267	72909	1.63%	0.160%
46	14.797	1110	1112	1116	rBV	204423	334815	7.47%	0.736%
47	14.888	1118	1120	1123	rVB	95890	108367	2.42%	0.238%
48	15.060	1133	1135	1138	rBV	111567	128963	2.88%	0.283%
49	15.117	1138	1140	1142	rVB	170706	178922	3.99%	0.393%
50	15.174	1142	1145	1148	rBV	741174	864488	19.30%	1.899%
51	15.288	1153	1155	1159	rVB4	32113	58776	1.31%	0.129%
52	15.597	1180	1182	1183	rBV	37423	52370	1.17%	0.115%
53	15.780	1196	1198	1203	rVB5	37224	70617	1.58%	0.155%
54	16.145	1228	1230	1235	rVB5	35129	78712	1.76%	0.173%
55	16.442	1253	1256	1260	rVB2	73821	140126	3.13%	0.308%
56	16.820	1286	1289	1293	rVB	59029	116803	2.61%	0.257%
57	17.814	1374	1376	1385	rVB8	23811	90675	2.02%	0.199%

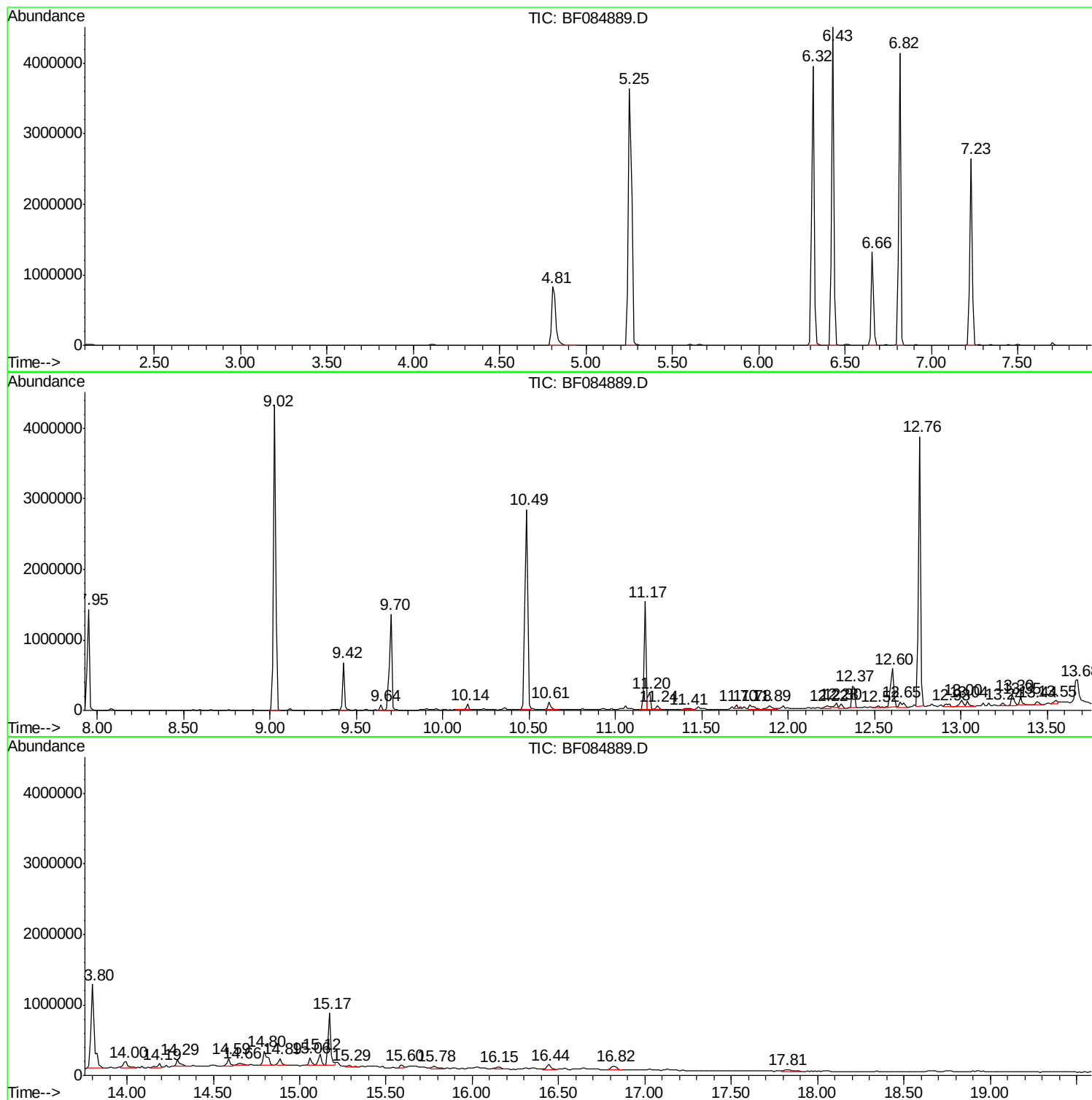
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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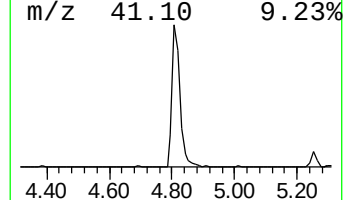
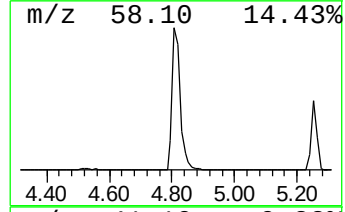
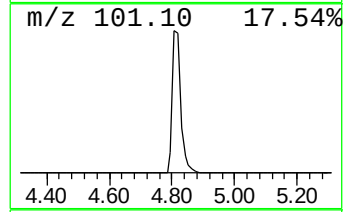
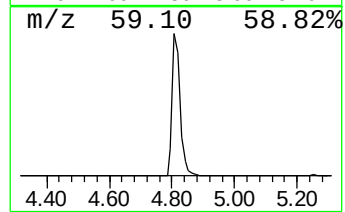
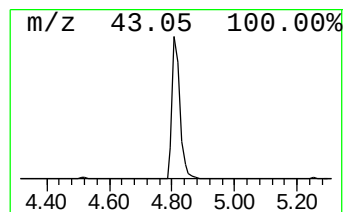
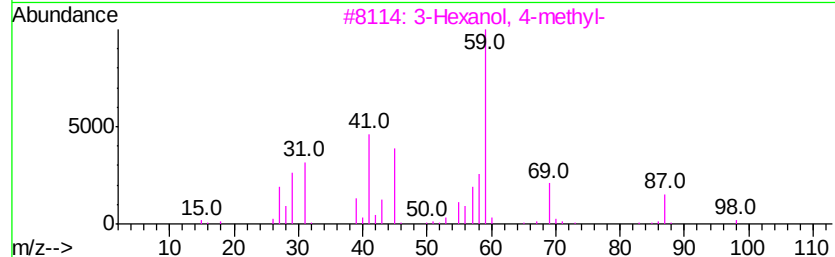
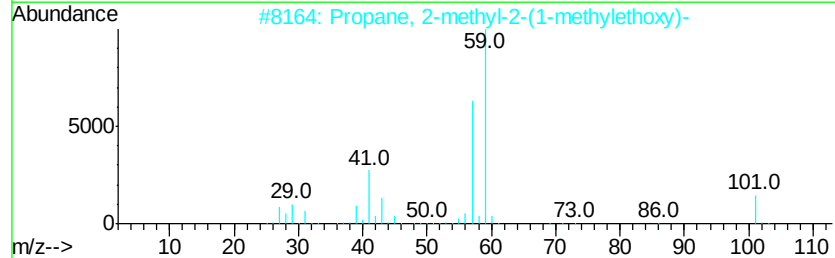
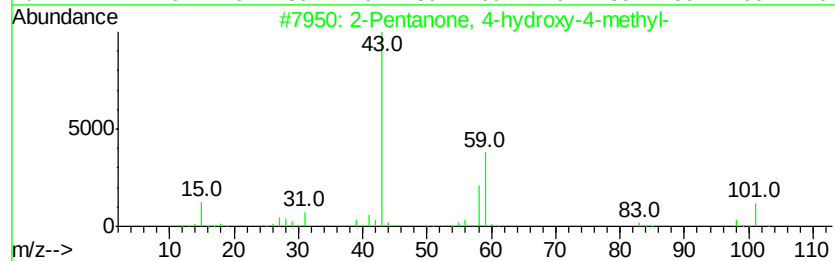
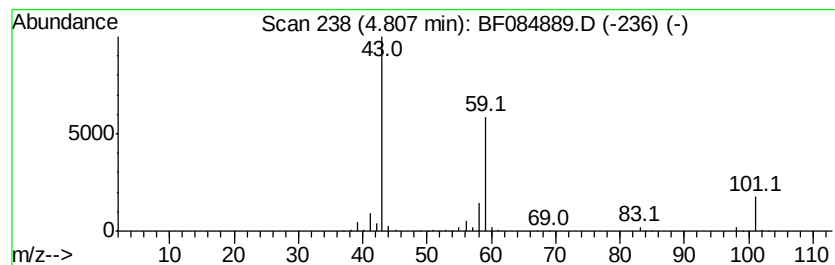
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	26.58 ng	1415660	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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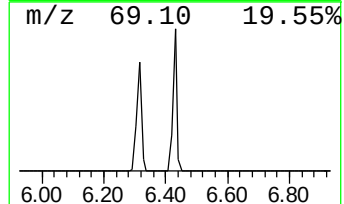
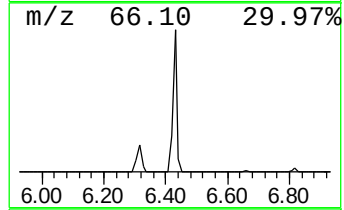
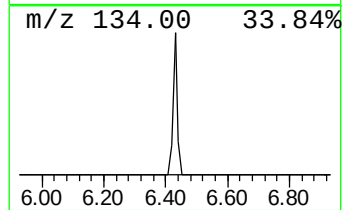
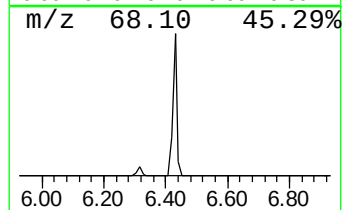
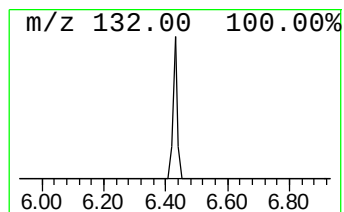
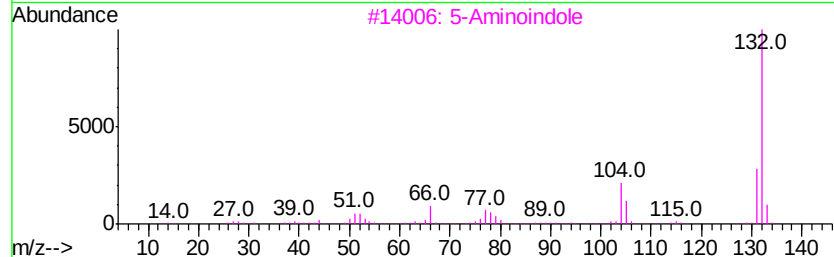
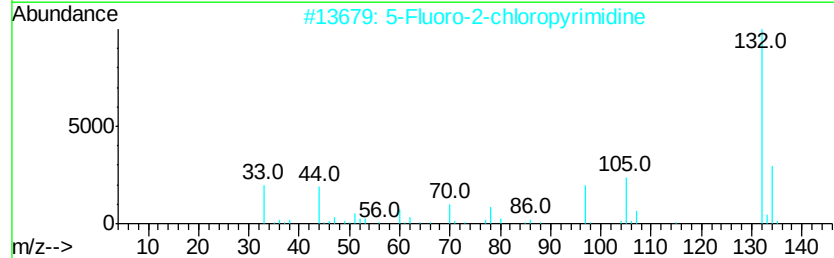
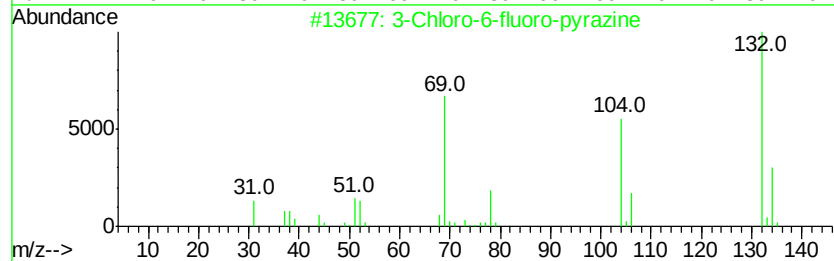
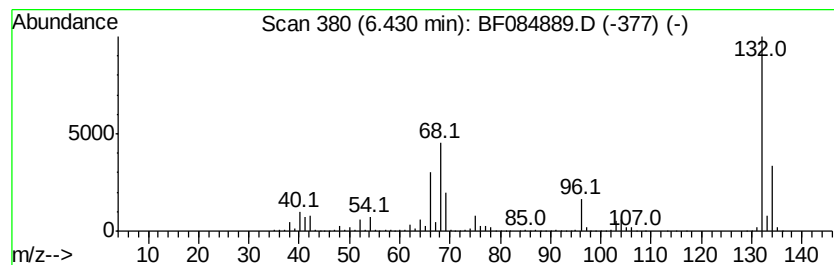
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.43 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	81.42 ng	4336080	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Xenon	132	Xe	007440-63-3	9



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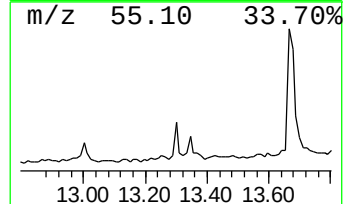
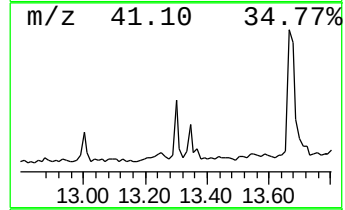
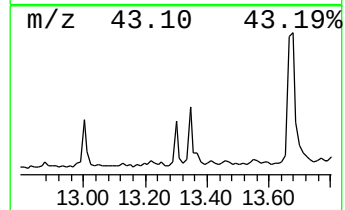
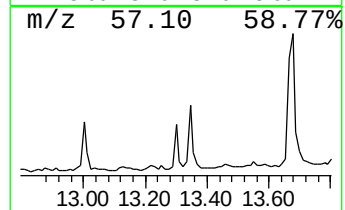
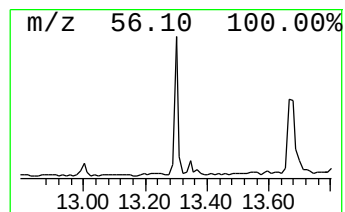
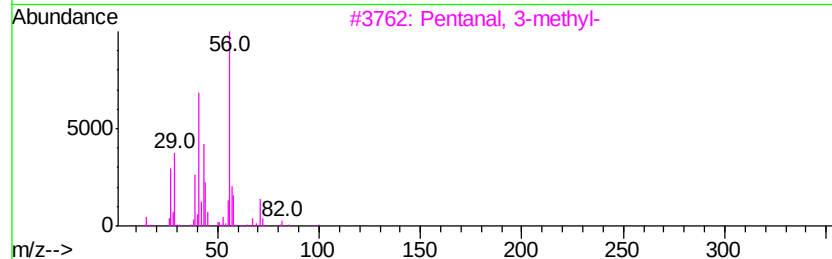
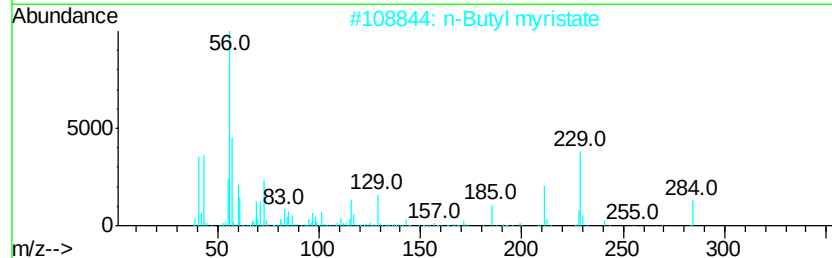
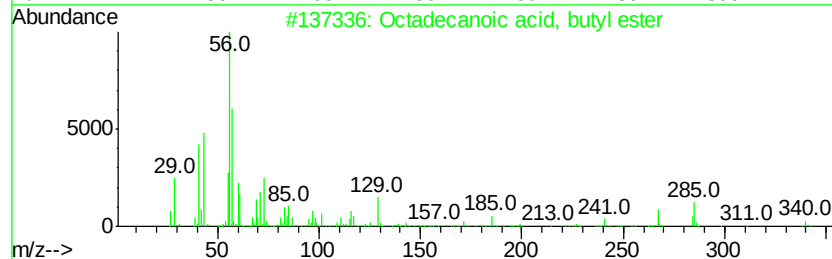
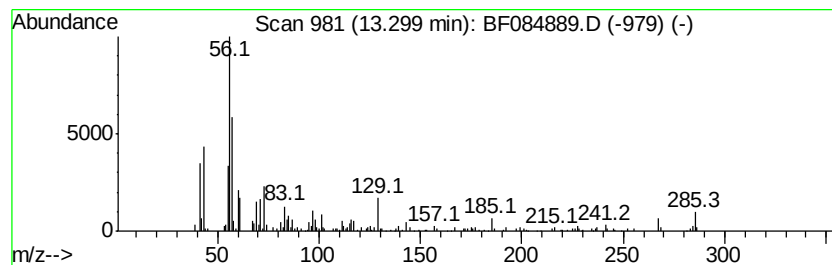
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.30	2.17 ng	158359	Chrysene-d12		13.80	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		n-Butyl myristate	284	C18H36O2	000110-36-1	86
3		Pentanal, 3-methyl-	100	C6H12O	015877-57-3	38
4		Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	38
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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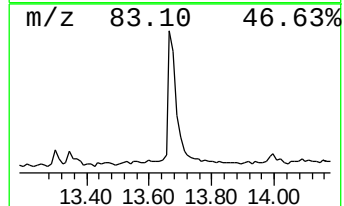
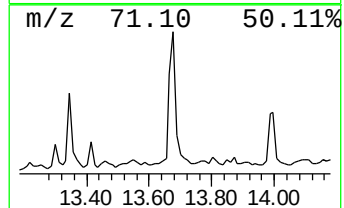
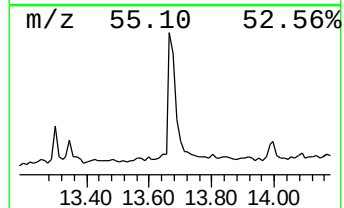
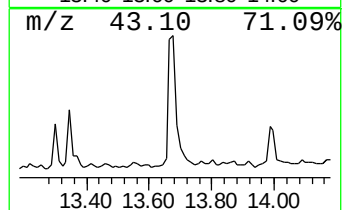
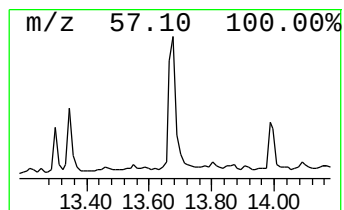
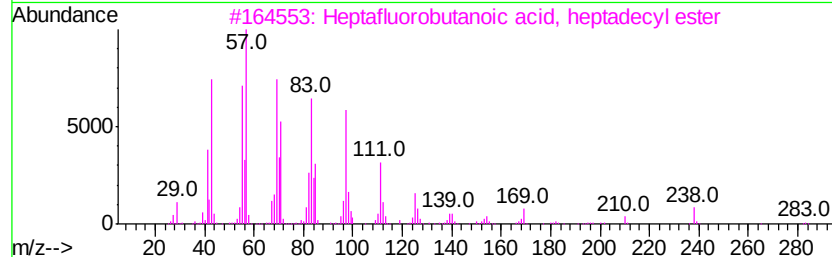
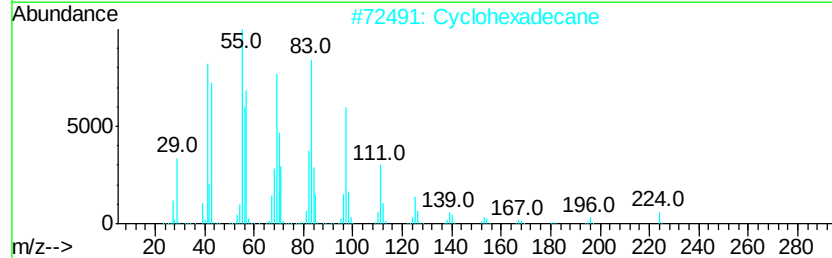
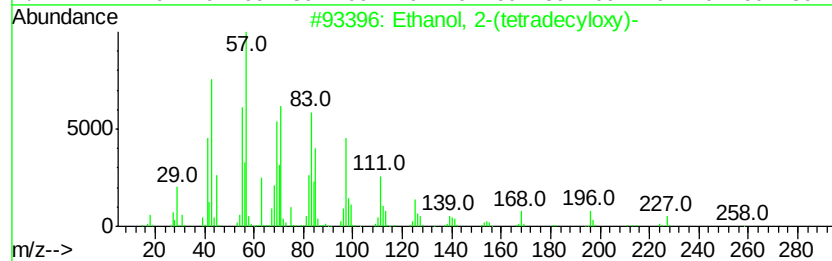
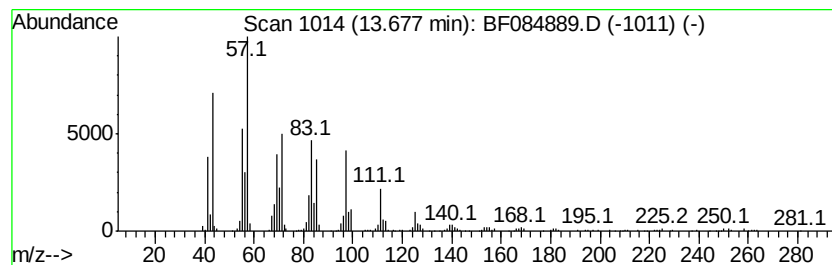
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.68	8.87 ng	648845	Chrysene-d12	13.80		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	80
2		Cyclohexadecane	224	C16H32	000295-65-8	78
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	74
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	72
5		17-Pentatriacontene	491	C35H70	006971-40-0	68



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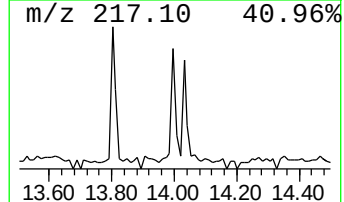
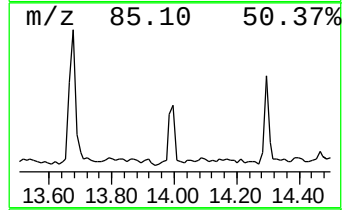
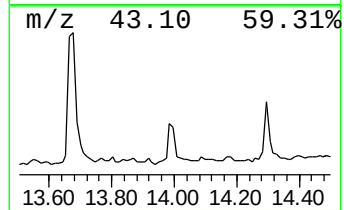
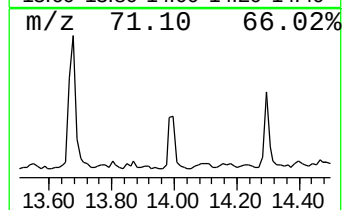
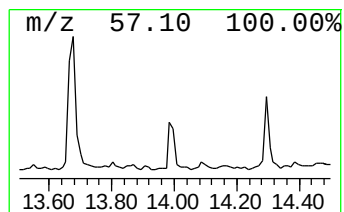
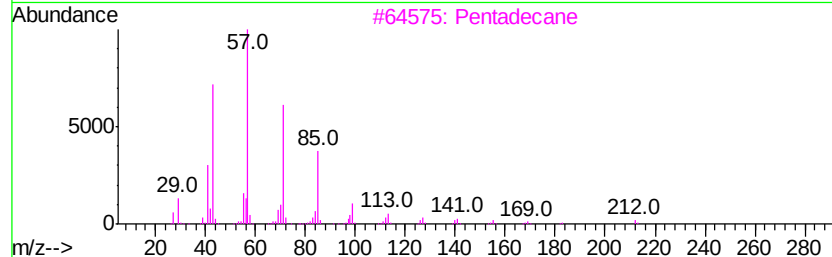
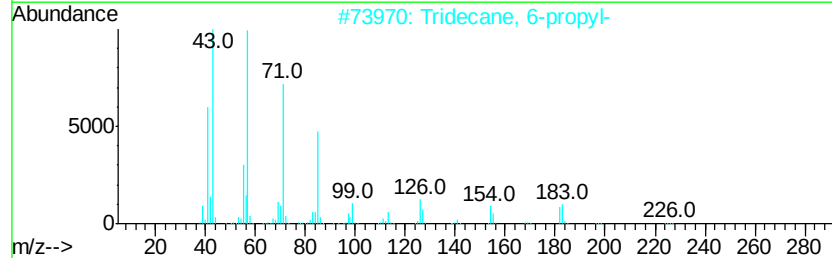
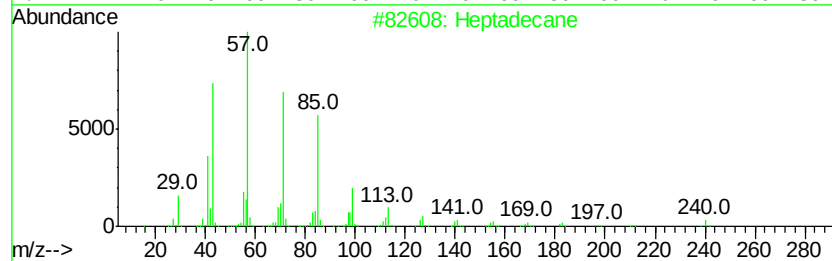
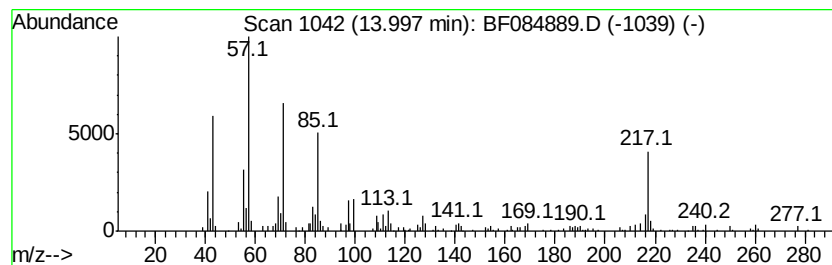
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	2.17 ng	158471	Chrysene-d12	13.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	78
2	Tridecane, 6-propyl-		226	C16H34	055045-10-8	53
3	Pentadecane		212	C15H32	000629-62-9	53
4	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	53
5	Hentriacontane		437	C31H64	000630-04-6	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084889.D
Acq On : 6 Feb 2016 4:50
Operator : SJ/IZ
Sample : H1329-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B006(21.5-23.5)

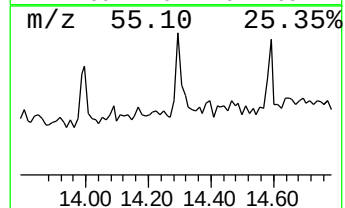
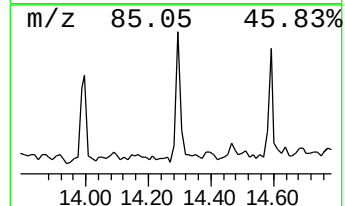
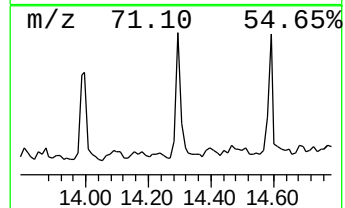
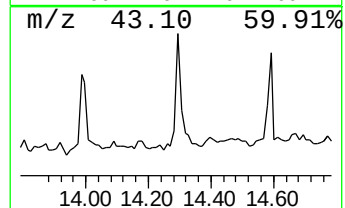
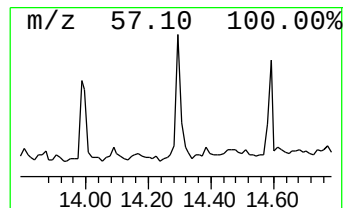
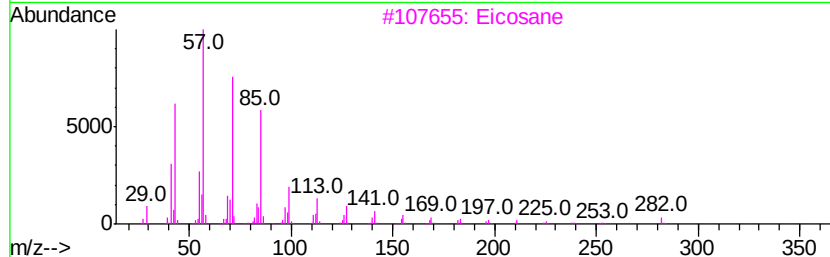
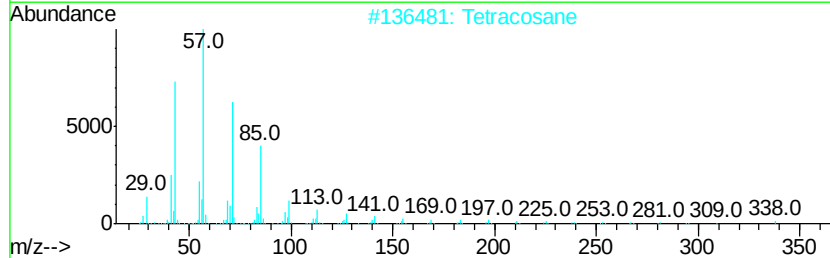
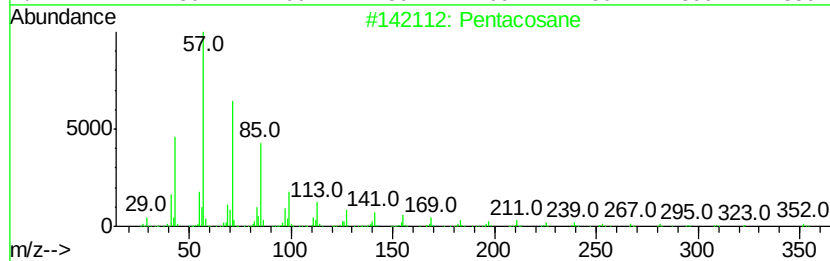
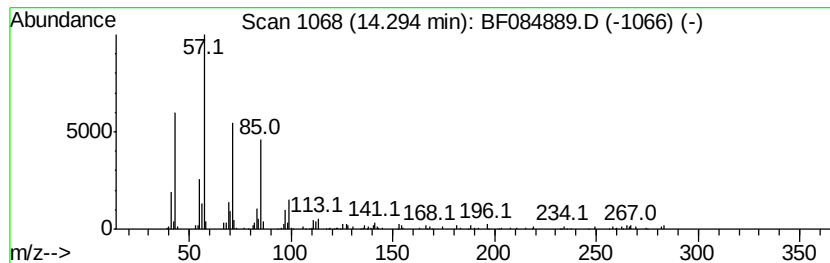
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.20 ng	161211	Chrysene-d12	13.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	86
2		Tetracosane	338	C24H50	000646-31-1	86
3		Eicosane	282	C20H42	000112-95-8	83
4		10-Methylnonadecane	282	C20H42	056862-62-5	74
5		Hexatriacontane	507	C36H74	000630-06-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084889.D
Acq On : 6 Feb 2016 4:50
Operator : SJ/IZ
Sample : H1329-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

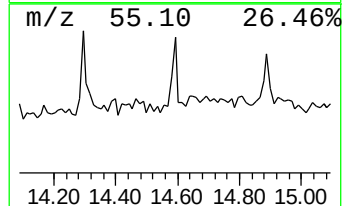
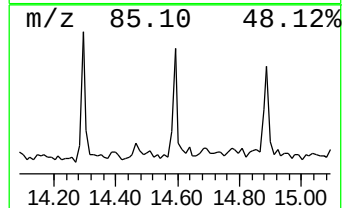
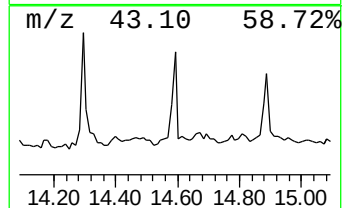
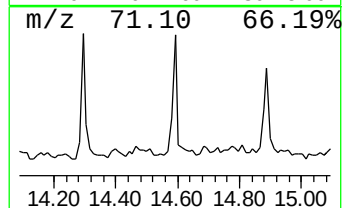
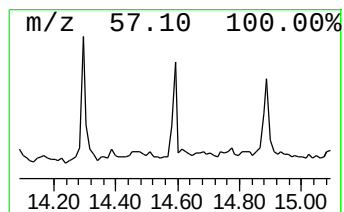
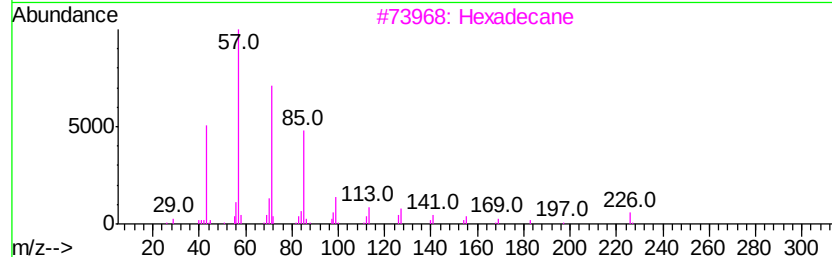
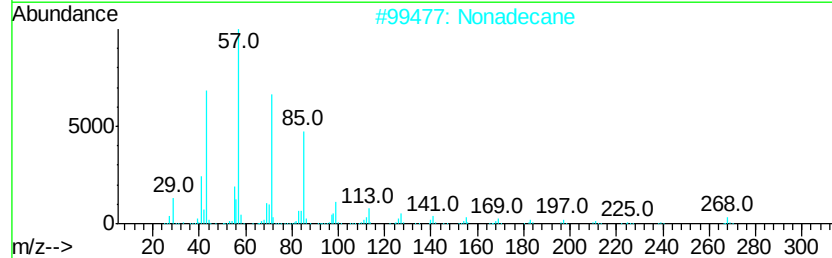
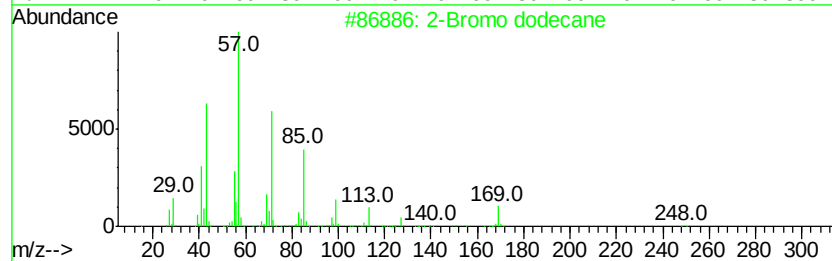
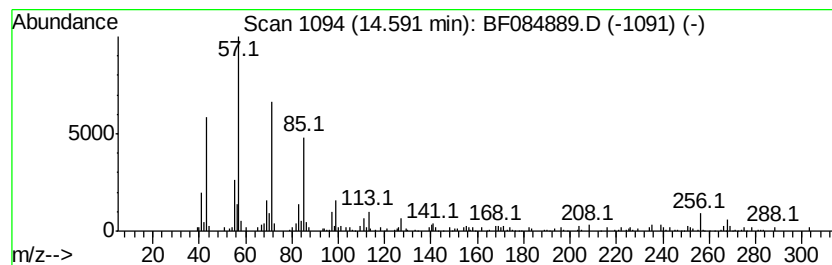
Instrument :
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ClientSampleId :
S4-B006(21.5-23.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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-Bromo dodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.59	3.00 ng	129530	Perylene-d12		15.17
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
2	Nonadecane	268	C19H40	000629-92-5	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Hentriacontane	437	C31H64	000630-04-6	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020516\
Data File : BF084889.D
Acq On : 6 Feb 2016 4:50
Operator : SJ/IZ
Sample : H1329-06
Misc :
ALS Vial : 34 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S4-B006(21.5-23.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020116.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...	4.81	26.6	ng	1415660	1	6.66	1065050	20.0
unknown6.43	6.43	81.4	ng	4336080	1	6.66	1065050	20.0
Octadecanoic acid...	13.30	2.2	ng	158359	5	13.80	1462590	20.0
Ethanol, 2-(tetra...	13.68	8.9	ng	648845	5	13.80	1462590	20.0
Heptadecane	14.00	2.2	ng	158471	5	13.80	1462590	20.0
Pentacosane	14.29	2.2	ng	161211	5	13.80	1462590	20.0
2-Bromo dodecane	14.59	3.0	ng	129530	6	15.17	864488	20.0