

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
 Data File : BF092381.D
 Acq On : 20 Jan 2017 19:13
 Operator : UM/SJ
 Sample : I1271-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-01

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-BF122116.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	4.621	246	248	260	rBV	757990	1454511	30.00%	3.601%
2	5.101	288	290	300	rBV	2370857	3381393	69.74%	8.372%
3	6.199	383	386	388	rBV	3053233	3723581	76.79%	9.219%
4	6.290	392	394	397	rVB	2491845	3376706	69.64%	8.360%
5	6.519	412	414	416	rBV	868604	823436	16.98%	2.039%
6	6.679	425	428	430	rBV	2820090	2656622	54.79%	6.577%
7	7.067	455	462	463	rBV	83885	138242	2.85%	0.342%
8	7.102	463	465	467	rVB	2665272	2931054	60.45%	7.257%
9	7.307	480	483	484	rBV2	58540	81489	1.68%	0.202%
10	7.445	492	495	497	rBV4	52984	99808	2.06%	0.247%
11	7.547	503	504	506	rBV2	50548	63969	1.32%	0.158%
12	7.639	510	512	514	rVB2	29891	50106	1.03%	0.124%
13	7.696	514	517	520	rBV2	30479	64977	1.34%	0.161%
14	7.810	525	527	529	rVV	1835551	1628839	33.59%	4.033%
15	7.890	533	534	538	rVB2	73632	95453	1.97%	0.236%
16	8.005	540	544	548	rBV5	30898	102865	2.12%	0.255%
17	8.096	548	552	555	rBV4	46392	133200	2.75%	0.330%
18	8.199	560	561	563	rVB2	46244	50386	1.04%	0.125%
19	8.256	563	566	570	rBV2	122688	188837	3.89%	0.468%
20	8.439	578	582	583	rBV4	37341	94545	1.95%	0.234%
21	8.622	596	598	601	rBV2	51665	99101	2.04%	0.245%
22	8.725	603	607	609	rBV4	35601	82389	1.70%	0.204%
23	8.850	615	618	619	rBV	146420	170942	3.53%	0.423%
24	8.896	619	622	624	rVV	4641071	4848739	100.00%	12.005%
25	8.988	624	630	632	rVV4	44972	111268	2.29%	0.275%
26	9.033	632	634	638	rVB2	46275	73594	1.52%	0.182%
27	9.148	642	644	646	rBV	67418	105624	2.18%	0.262%
28	9.228	649	651	652	rBV	78482	103361	2.13%	0.256%
29	9.262	652	654	655	rVB2	62241	79115	1.63%	0.196%
30	9.296	655	657	659	rBV	533476	538334	11.10%	1.333%
31	9.422	666	668	669	rBV2	47553	65600	1.35%	0.162%
32	9.468	670	672	674	rVB3	53957	65555	1.35%	0.162%
33	9.513	674	676	677	rBV	70146	71869	1.48%	0.178%
34	9.559	677	680	682	rVV	1627013	1543984	31.84%	3.823%

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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	9.605	682	684	687 rVV2	37578	69917	1.44%	0.173%
36	9.673	687	690	692 rVB2	53716	88839	1.83%	0.220%
37	9.765	695	698	700 rVV2	87573	115428	2.38%	0.286%
38	9.799	700	701	703 rVB	49877	64863	1.34%	0.161%
39	9.833	703	704	706 rVB2	74742	63269	1.30%	0.157%
40	9.879	706	708	713 rBV2	78944	172464	3.56%	0.427%
41	9.959	713	715	718 rBV3	57963	118163	2.44%	0.293%
42	10.005	718	719	721 rVB	74350	81330	1.68%	0.201%
43	10.233	736	739	740 rBV	108564	148777	3.07%	0.368%
44	10.348	747	749	752 rBV	2269740	2236958	46.13%	5.538%
45	10.496	759	762	764 rVB2	183431	339618	7.00%	0.841%
46	10.679	776	778	779 rBV2	66924	64224	1.32%	0.159%
47	10.931	798	800	801 rBV	92326	116203	2.40%	0.288%
48	10.953	801	802	805 rVB	136037	125862	2.60%	0.312%
49	11.033	807	809	813 rBV	1384638	1267268	26.14%	3.138%
50	11.353	835	837	839 rBV2	99036	107294	2.21%	0.266%
51	11.536	851	853	856 rBV3	30811	52385	1.08%	0.130%
52	11.594	856	858	861 rBV	195759	220303	4.54%	0.545%
53	11.754	871	872	876 rVB	59769	79376	1.64%	0.197%
54	12.085	899	901	903 rBV2	51469	78848	1.63%	0.195%
55	12.245	913	915	917 rBV	54867	68928	1.42%	0.171%
56	12.371	925	926	930 rBV4	75988	140390	2.90%	0.348%
57	12.462	932	934	938 rBV3	61201	159690	3.29%	0.395%
58	12.622	945	948	950 rBV	3590836	3459690	71.35%	8.566%
59	12.896	971	972	976 rVB	95438	100332	2.07%	0.248%
60	13.662	1037	1039	1042 rBV	997639	1093763	22.56%	2.708%
61	15.022	1155	1158	1160 rBV	460300	656804	13.55%	1.626%

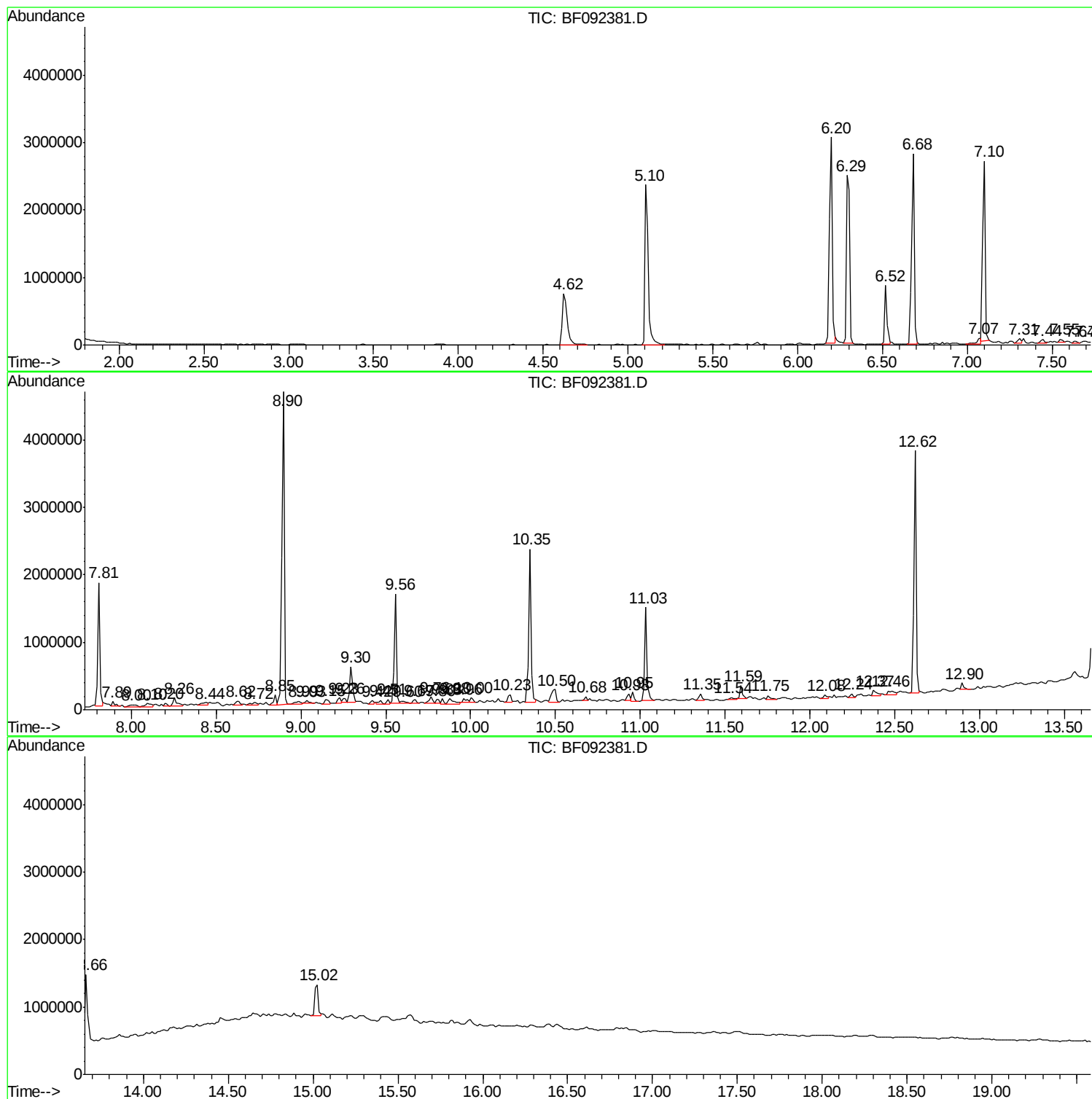
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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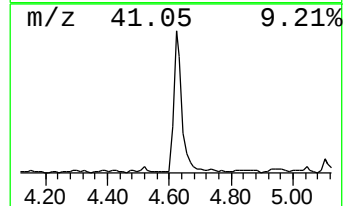
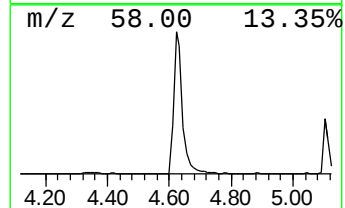
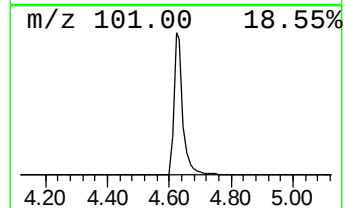
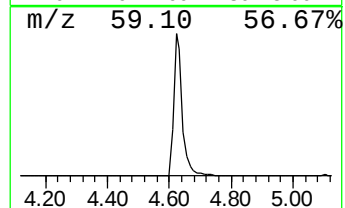
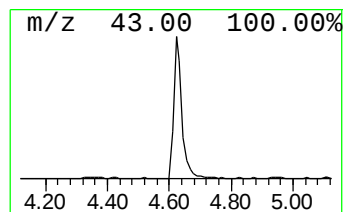
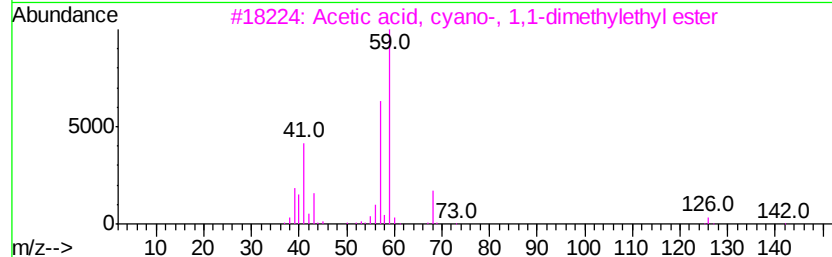
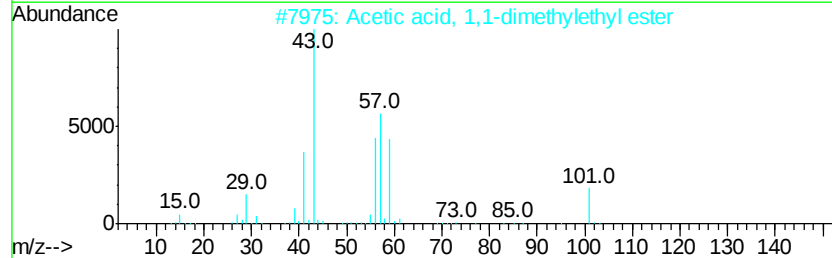
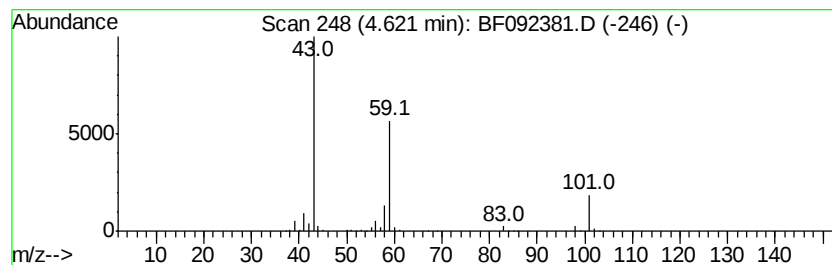
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	35.33 ng	1454510	1,4-Dichlorobenzene-d4	6.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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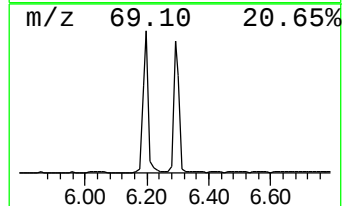
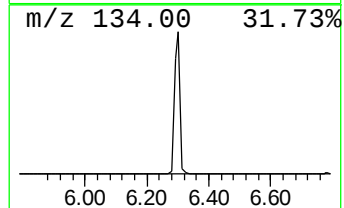
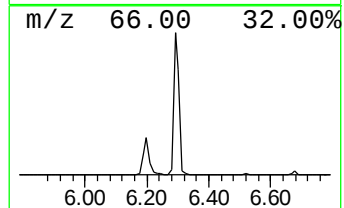
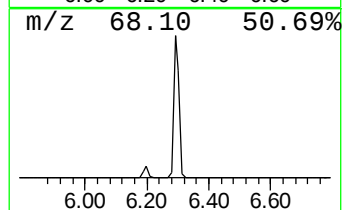
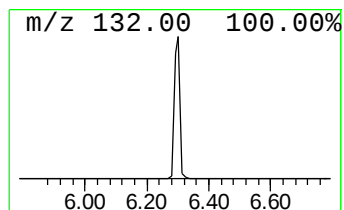
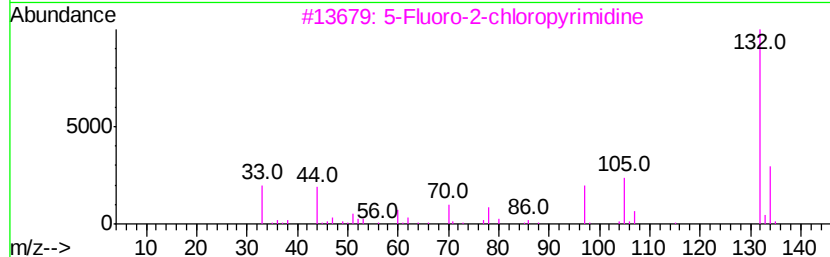
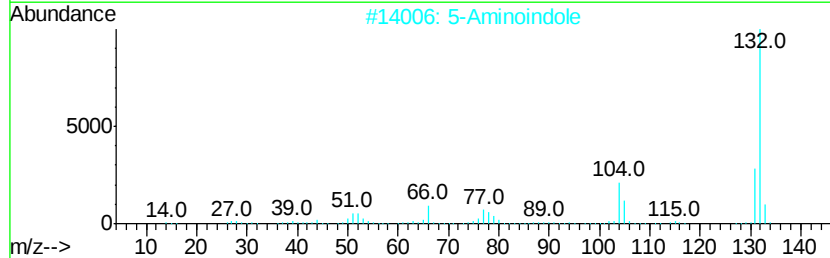
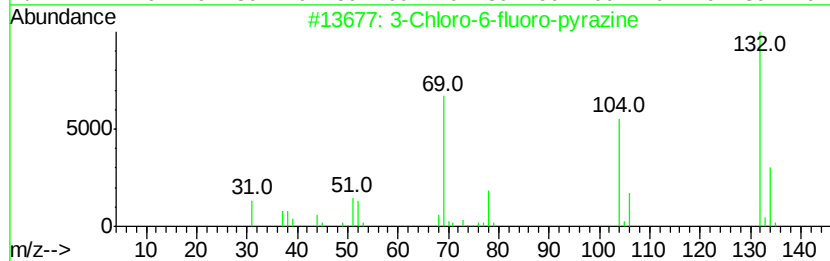
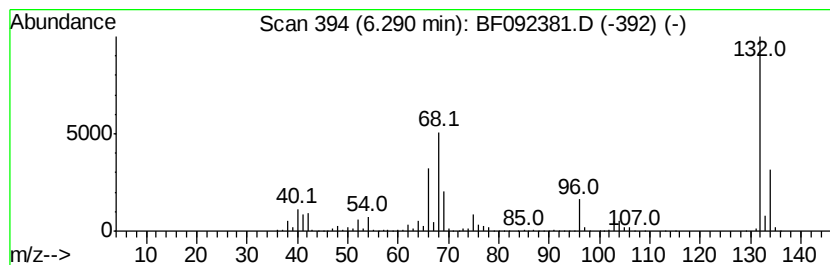
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.29	82.02 ng	3376710	1,4-Dichlorobenzene-d4	6.52

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Aminoindole	132	C8H8N2	005192-03-0	22
3	5		Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	2		Cyclohexen-1-one	96	C6H8O	000930-68-7	11
5			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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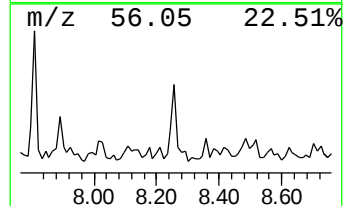
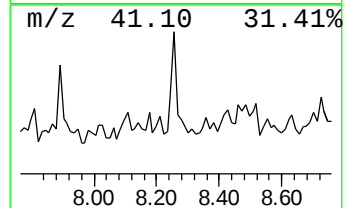
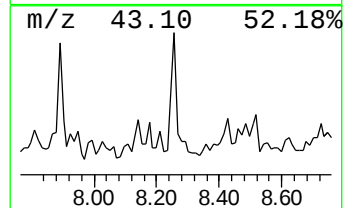
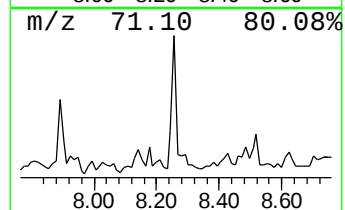
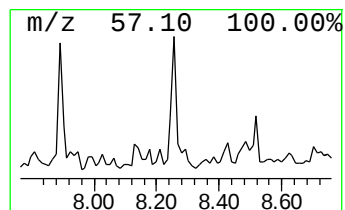
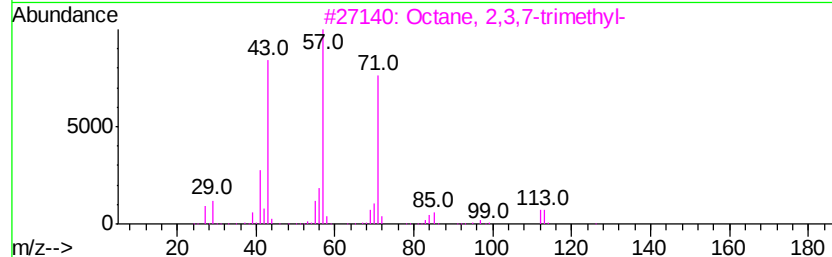
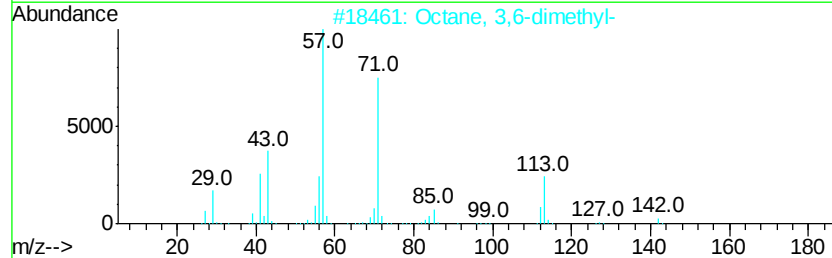
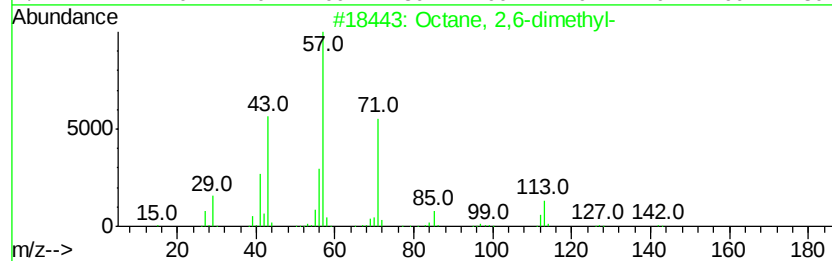
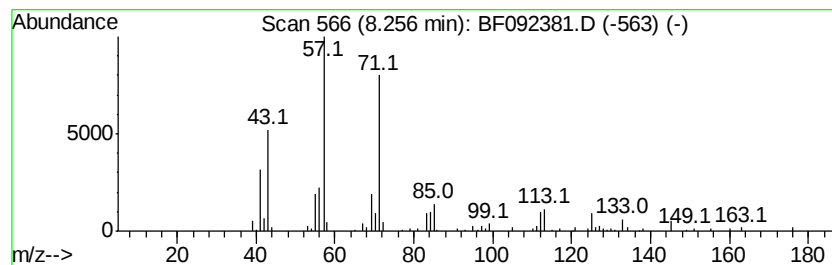
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octane, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	2.32 ng	188837	Napthalene-d8	7.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	72
2		Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64
3		Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	59
4		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	50
5		Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	50



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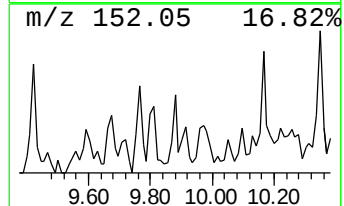
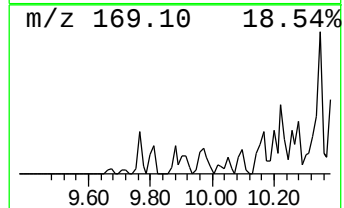
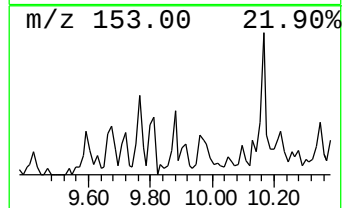
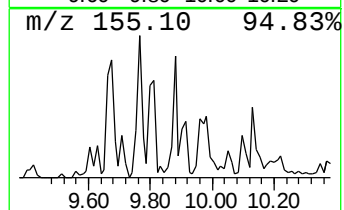
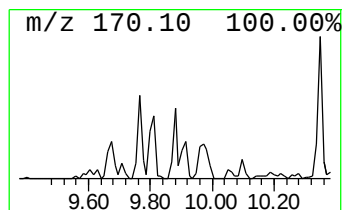
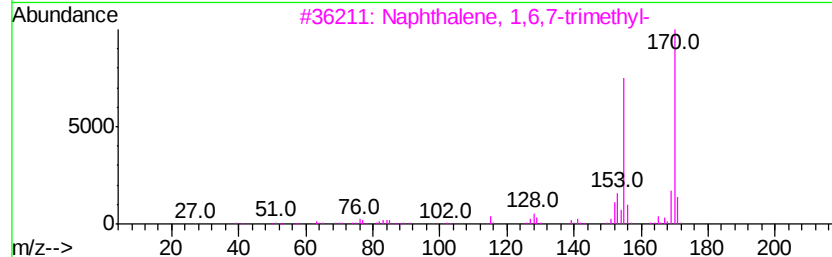
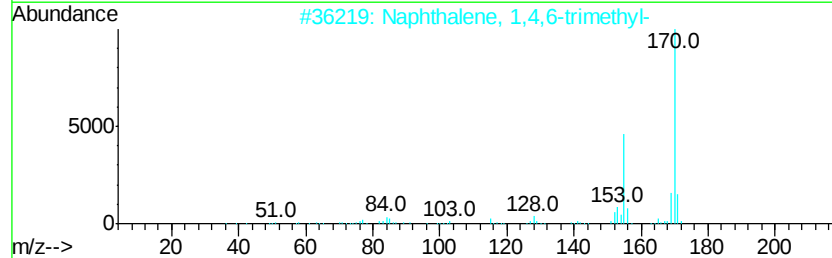
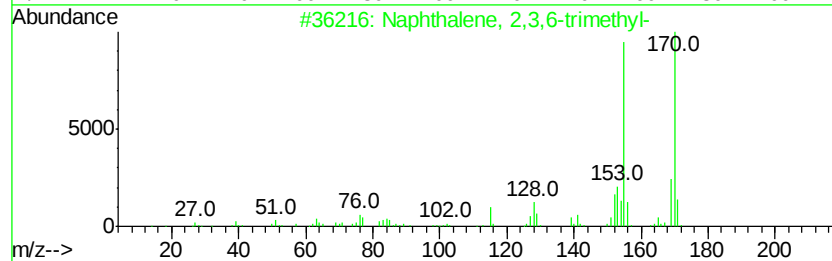
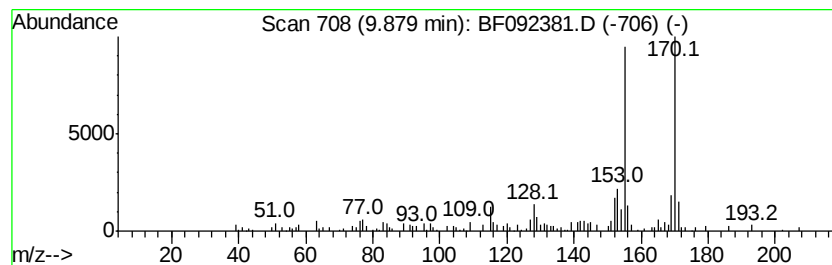
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Naphthalene, 2,3,6-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.88	2.23 ng	172464	Acenaphthene-d10	9.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	98
2		Naphthalene, 1,4,6-trimethyl-	170	C13H14	002131-42-2	97
3		Naphthalene, 1,6,7-trimethyl-	170	C13H14	002245-38-7	96
4		Naphthalene, 1,4,5-trimethyl-	170	C13H14	002131-41-1	96
5		Azulene, 4,6,8-trimethyl-	170	C13H14	000941-81-1	94



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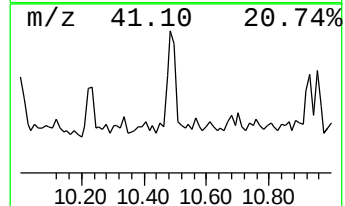
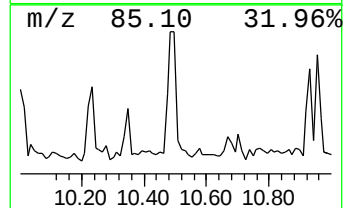
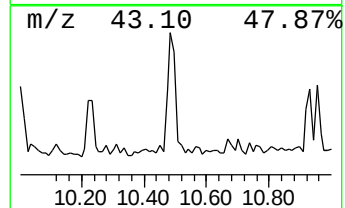
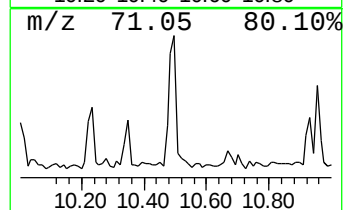
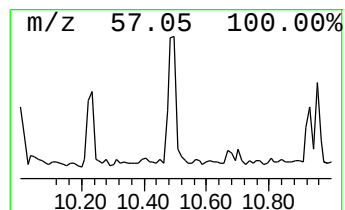
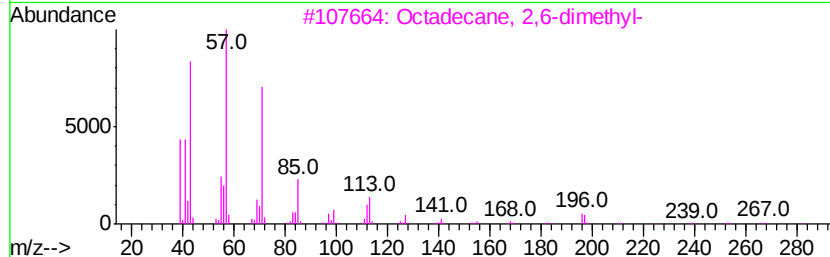
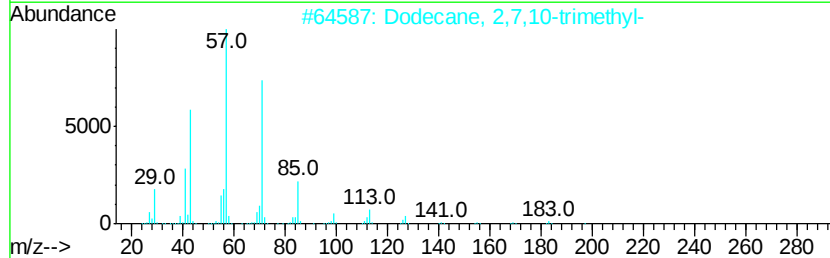
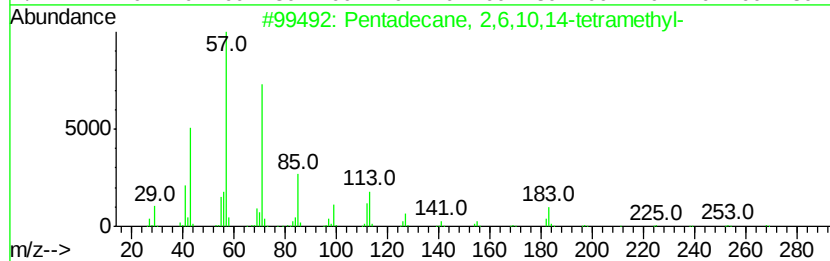
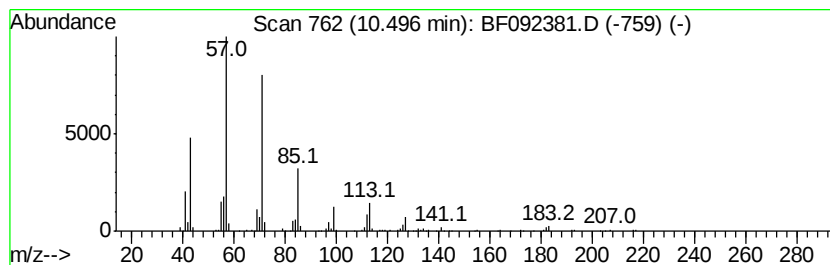
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecane, 2,6,10,14-tetr... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	5.36 ng	339618	Phenanthrene-d10	11.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	90
2		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3		Octadecane, 2,6-dimethyl-	282	C20H42	075163-97-2	83
4		Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	78
5		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092381.D
Acq On : 20 Jan 2017 19:13
Operator : UM/SJ
Sample : I1271-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-01

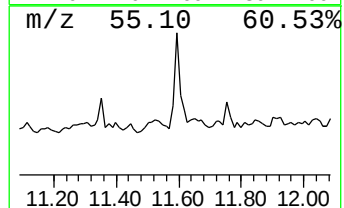
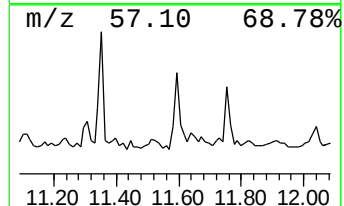
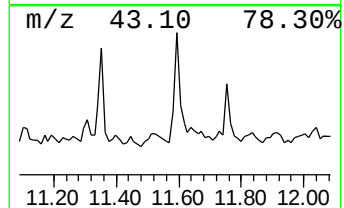
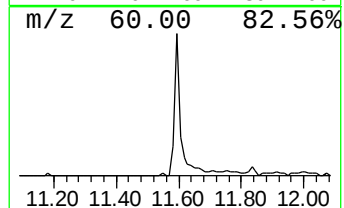
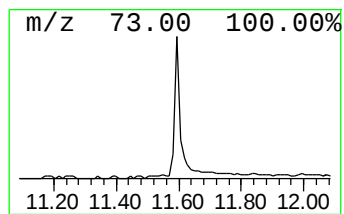
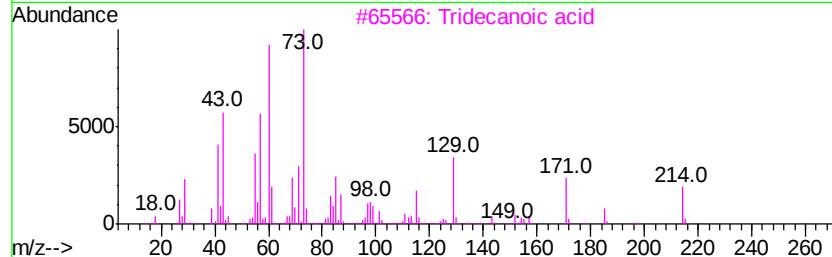
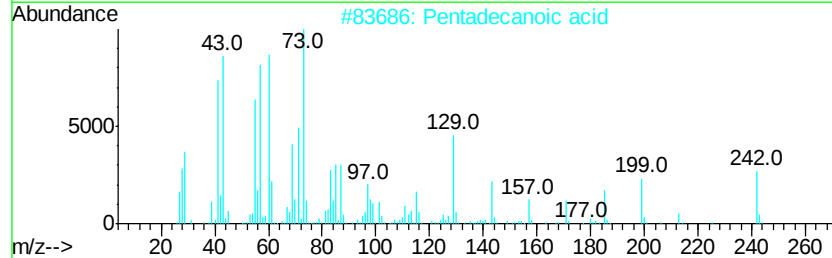
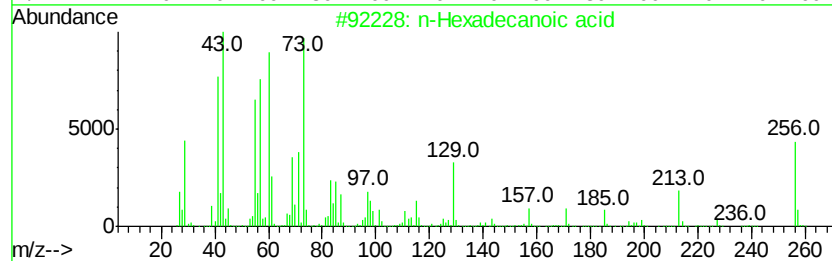
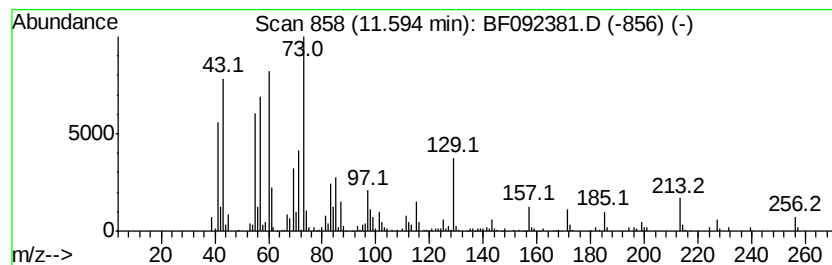
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	3.48 ng	220303	Phenanthrene-d10	11.03

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	49
5		Nonanoic acid	158	C9H18O2	000112-05-0	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012017\
Data File : BF092381.D
Acq On : 20 Jan 2017 19:13
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Sample : I1271-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-01

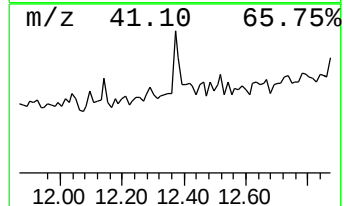
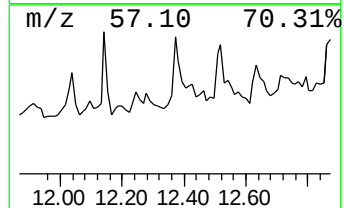
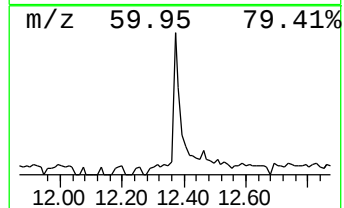
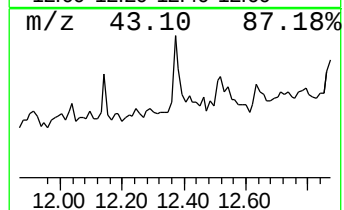
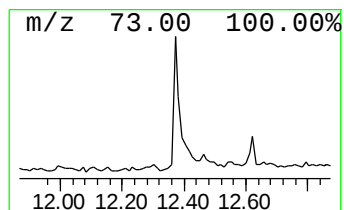
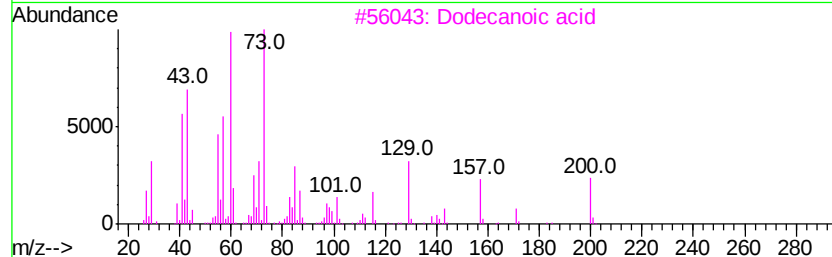
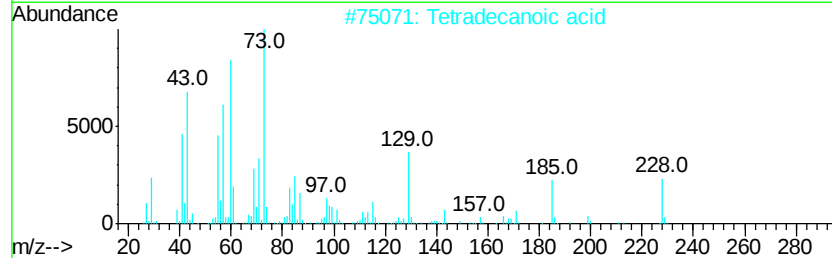
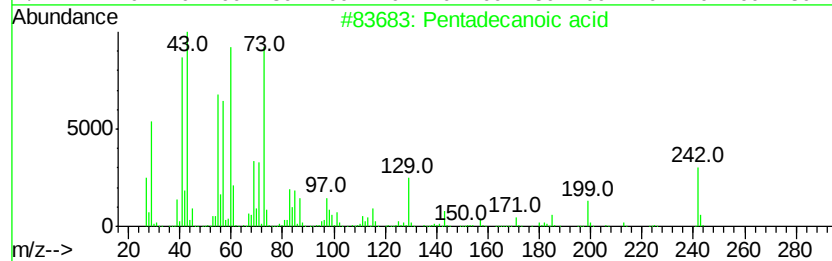
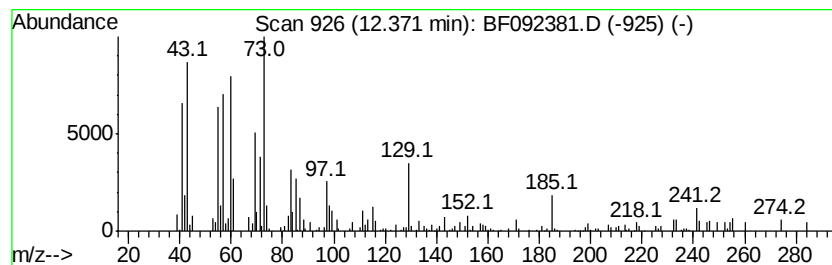
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	2.57 ng	140390	Chrysene-d12	13.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3		Dodecanoic acid	200	C12H24O2	000143-07-7	59
4		.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	53
5		Tridecanoic acid	214	C13H26O2	000638-53-9	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012017\
Data File : BF092381.D
Acq On : 20 Jan 2017 19:13
Operator : UM/SJ
Sample : I1271-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-01

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.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...	4.62	35.3	ng	1454510	1	6.52	823436	20.0
unknown6.29	6.29	82.0	ng	3376710	1	6.52	823436	20.0
Octane, 2,6-dimet...	8.26	2.3	ng	188837	2	7.81	1628840	20.0
Naphthalene, 2,3,...	9.88	2.2	ng	172464	3	9.56	1543980	20.0
Pentadecane, 2,6,...	10.50	5.4	ng	339618	4	11.03	1267270	20.0
n-Hexadecanoic acid	11.59	3.5	ng	220303	4	11.03	1267270	20.0
Pentadecanoic acid	12.37	2.6	ng	140390	5	13.66	1093760	20.0