

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
 Data File : BF092460.D
 Acq On : 25 Jan 2017 5:37
 Operator : UM/SJ
 Sample : I1397-06
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W-27

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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	3.961	161	164	167	rBV	95707	141832	3.18%	0.426%
2	5.139	265	267	270	rBV	550271	619668	13.89%	1.859%
3	5.242	272	276	278	rVB	52248	56658	1.27%	0.170%
4	5.550	301	303	306	rBV	1879218	2006241	44.96%	6.019%
5	6.305	367	369	374	rBV	58508	78358	1.76%	0.235%
6	6.579	390	393	395	rBV	1596503	1345271	30.14%	4.036%
7	6.727	403	406	409	rBV	3333481	3330886	74.64%	9.994%
8	6.967	424	427	429	rBV	1110665	949595	21.28%	2.849%
9	7.127	438	441	443	rVB	3510255	3470628	77.77%	10.413%
10	7.367	459	462	464	rBV2	32005	54756	1.23%	0.164%
11	7.527	473	476	478	rBV	2106190	3043582	68.20%	9.132%
12	7.653	485	487	491	rVB	47299	64667	1.45%	0.194%
13	8.259	538	540	542	rVB	1469579	1237703	27.73%	3.713%
14	9.345	632	635	637	rBV	4657485	4462702	100.00%	13.389%
15	9.733	666	669	672	rBV2	139014	202710	4.54%	0.608%
16	9.916	682	685	688	rBV2	38097	49092	1.10%	0.147%
17	10.019	692	694	697	rVB	931026	1298380	29.09%	3.896%
18	10.156	703	706	708	rBV	59291	52586	1.18%	0.158%
19	10.316	716	720	722	rBV	75232	93025	2.08%	0.279%
20	10.442	729	731	738	rVB3	89683	121348	2.72%	0.364%
21	10.819	761	764	766	rBV	2441038	2644821	59.27%	7.935%
22	10.911	769	772	773	rBV	108605	96390	2.16%	0.289%
23	10.934	773	774	777	rVV2	41074	60411	1.35%	0.181%
24	11.036	781	783	784	rVB	38370	46574	1.04%	0.140%
25	11.174	794	795	797	rVB2	43789	56227	1.26%	0.169%
26	11.219	797	799	801	rBV	47136	61846	1.39%	0.186%
27	11.402	812	815	820	rVB2	107763	145899	3.27%	0.438%
28	11.516	823	825	827	rBV	1420386	1224904	27.45%	3.675%
29	11.745	841	845	846	rBV3	36689	48939	1.10%	0.147%
30	12.042	869	871	876	rBV4	110424	189258	4.24%	0.568%
31	12.225	885	887	891	rVB3	40512	75409	1.69%	0.226%
32	12.774	929	935	938	rBV8	20516	88223	1.98%	0.265%
33	12.831	938	940	947	rVB3	81774	120648	2.70%	0.362%
34	12.934	947	949	952	rBV2	62796	116425	2.61%	0.349%

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35	12.979	952	953	958	rVB2	69419	91458	2.05%	0.274%
36	13.105	961	964	967	rBV	3703329	3593593	80.53%	10.782%
37	13.631	1008	1010	1011	rBV	56664	50914	1.14%	0.153%
38	13.665	1011	1013	1015	rVB	79196	81646	1.83%	0.245%
39	13.997	1040	1042	1049	rVB	84938	123273	2.76%	0.370%
40	14.145	1053	1055	1058	rBV	808356	887143	19.88%	2.662%
41	15.620	1181	1184	1187	rBV	583544	846257	18.96%	2.539%

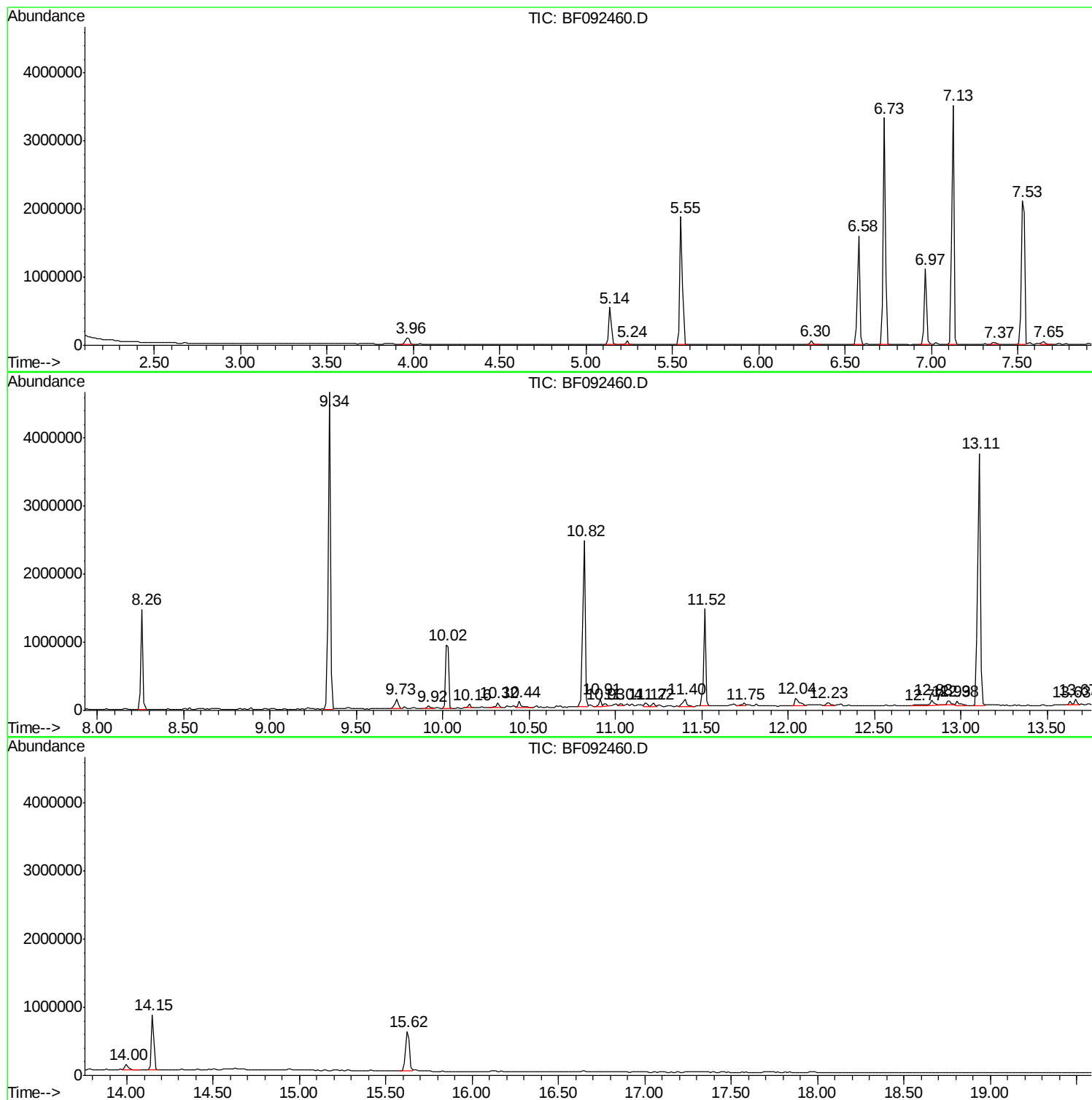
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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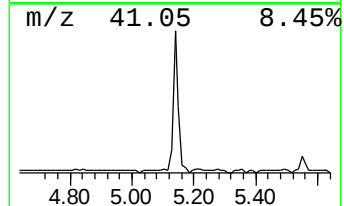
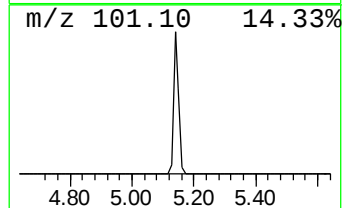
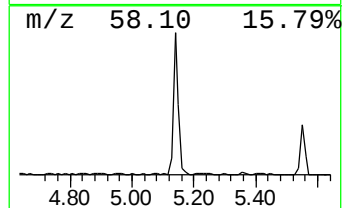
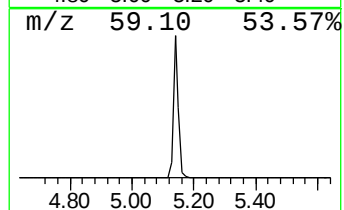
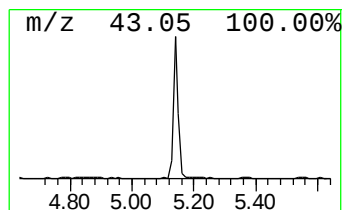
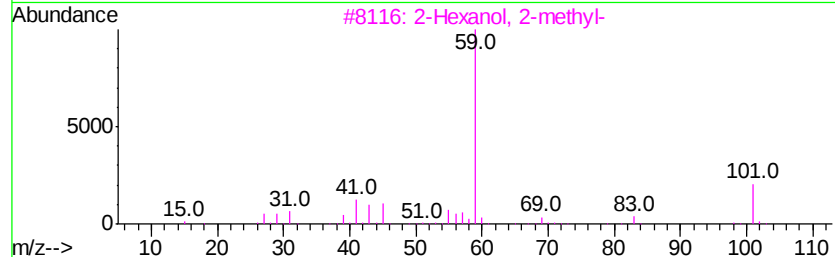
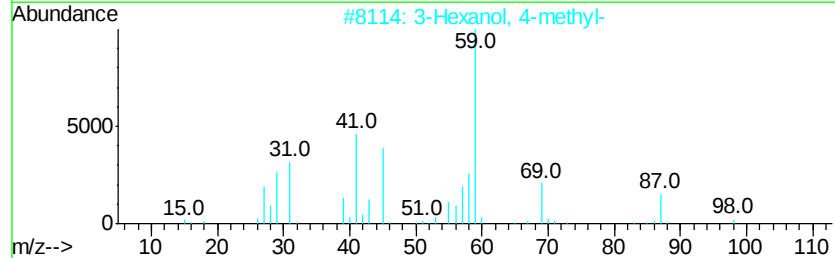
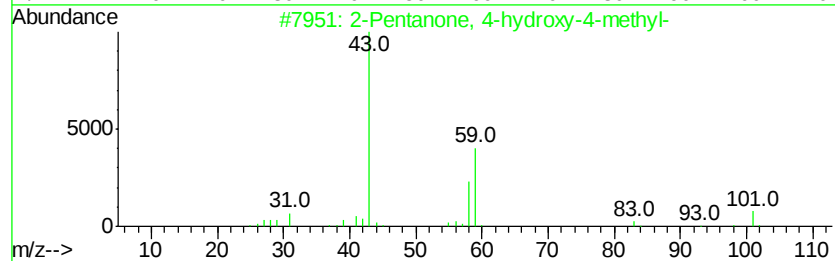
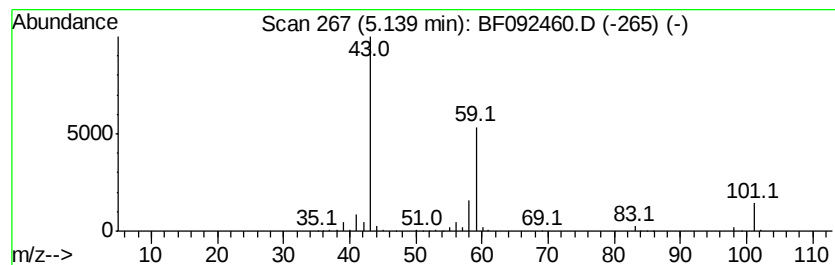
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	13.05 ng	619668	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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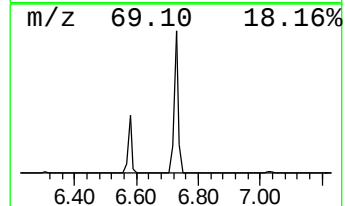
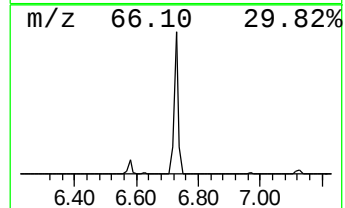
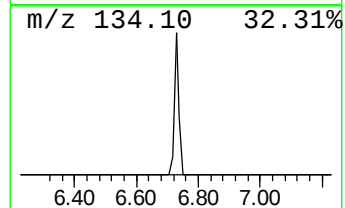
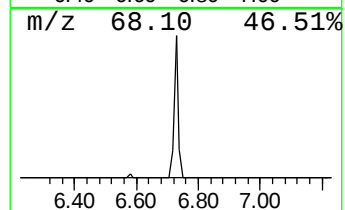
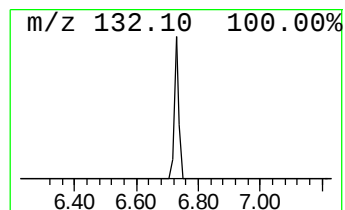
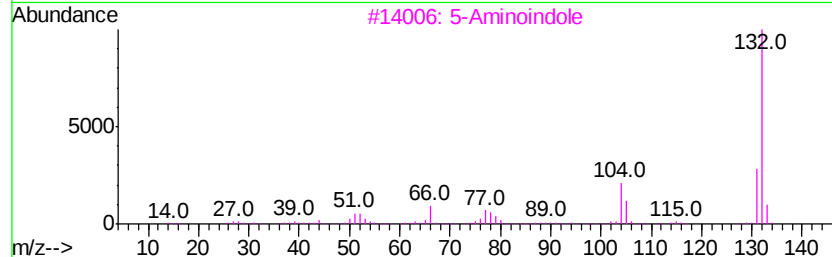
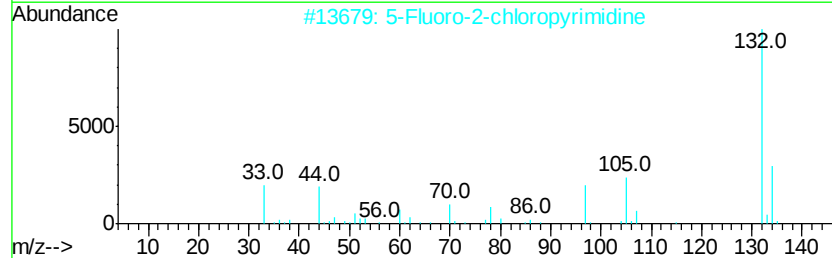
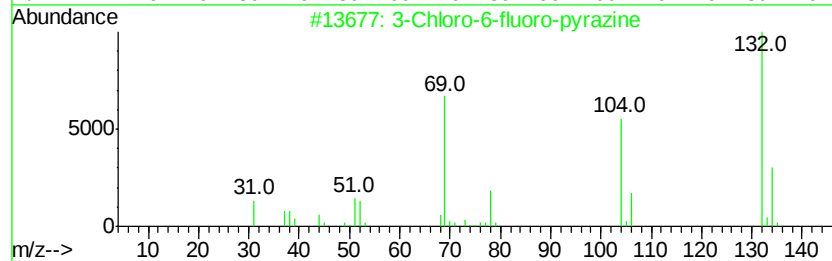
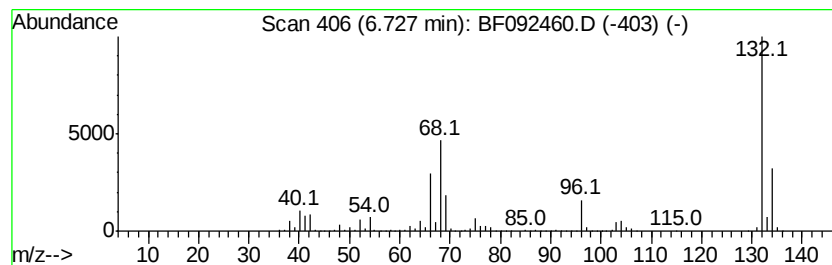
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	70.15 ng	3330890	1,4-Dichlorobenzene-d4	6.97

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	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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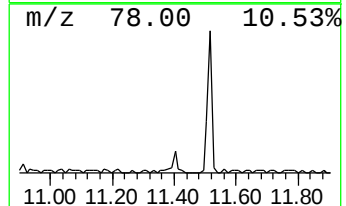
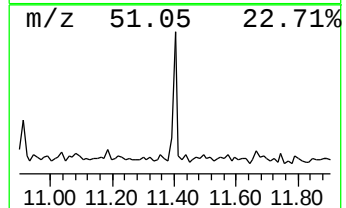
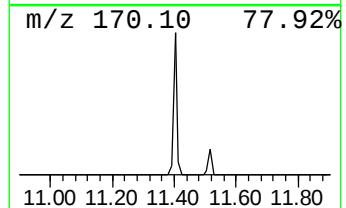
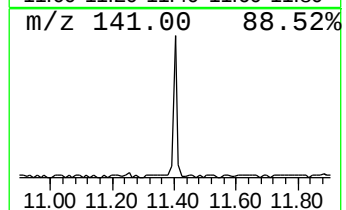
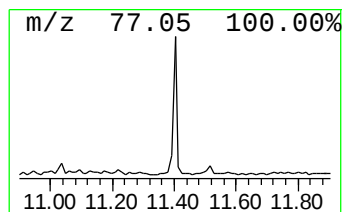
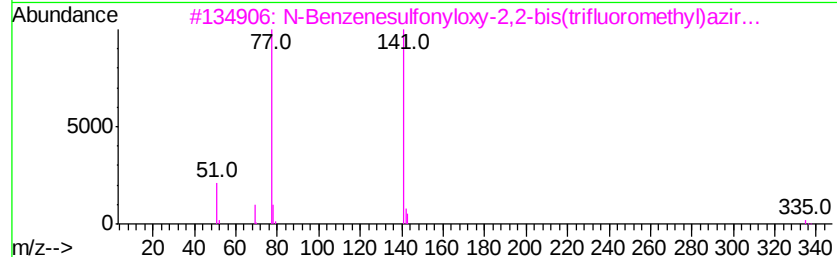
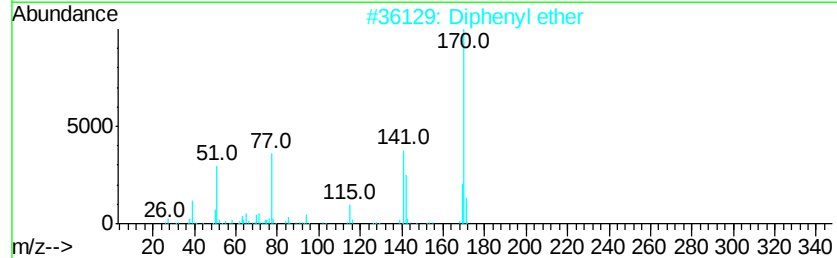
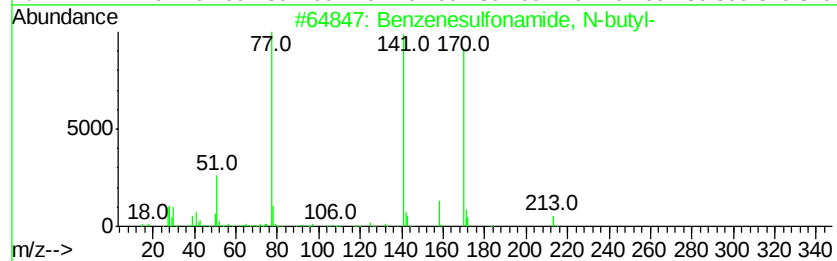
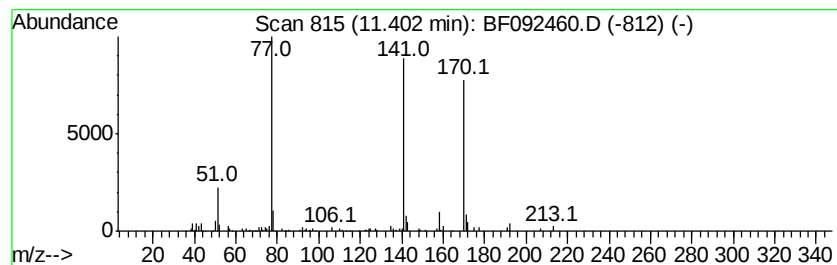
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Benzenesulfonamide, N-butyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	2.38 ng	145899	Phenanthrene-d10	11.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	95
2		Diphenyl ether	170	C12H10O	000101-84-8	56
3		N-Benzenesulfonyloxv-2,2-bis(tri...	335	C10H7F6N03S	055734-41-3	50
4		N,N-Dichlorobenzenesulfonamide	225	C6H5Cl2NO2S	000473-29-0	47
5		Benzenesulfonyl chloride	176	C6H5ClO2S	000098-09-9	47



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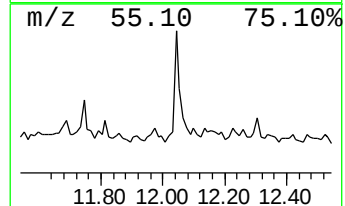
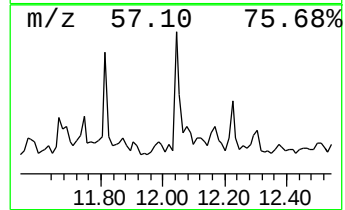
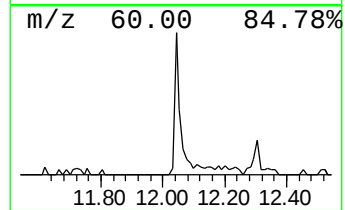
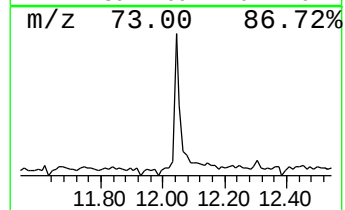
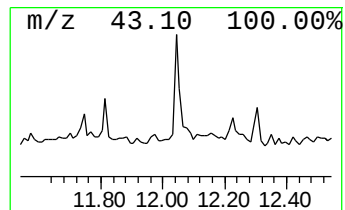
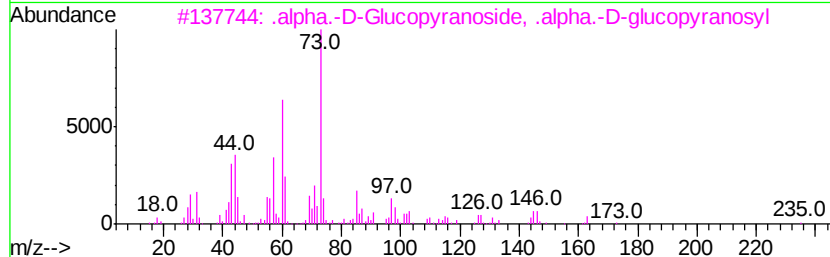
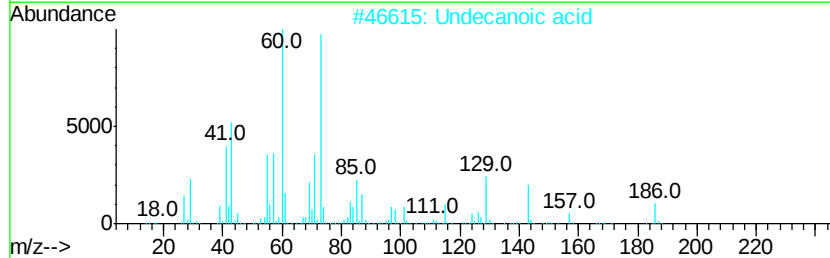
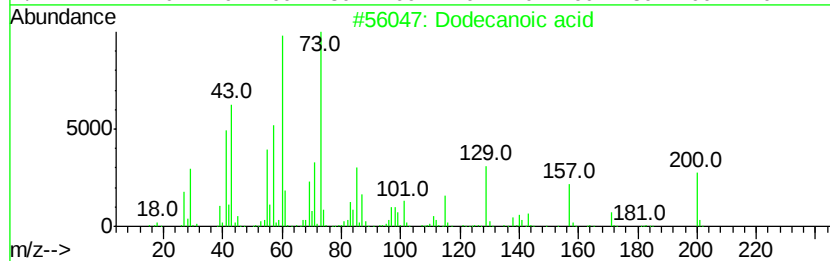
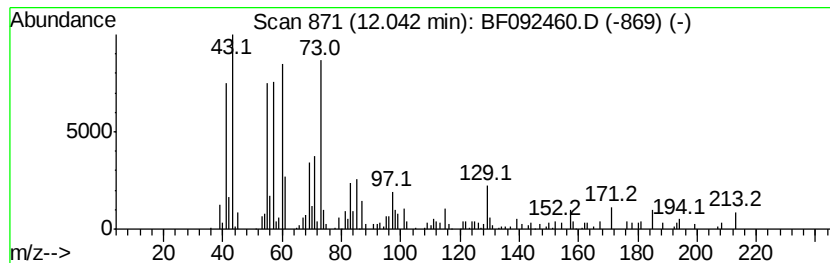
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Dodecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	3.09 ng	189258	Phenanthrene-d10	11.52

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	59	
2	Undecanoic acid	186	C11H22O2	000112-37-8	53	
3	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	50	
4	Butyraldehyde, semicarbazone	129	C5H11N3O	013183-21-6	49	
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	43	



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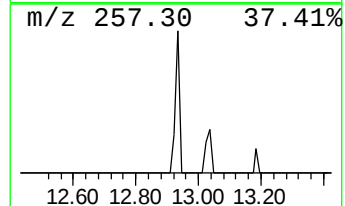
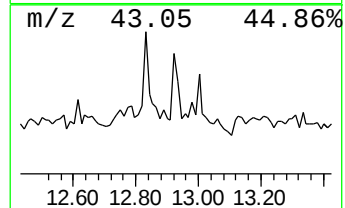
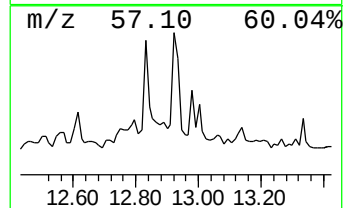
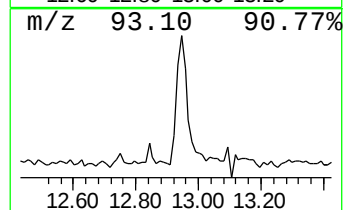
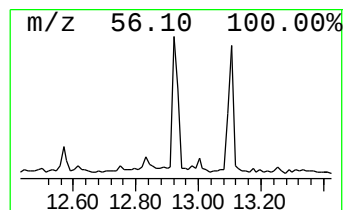
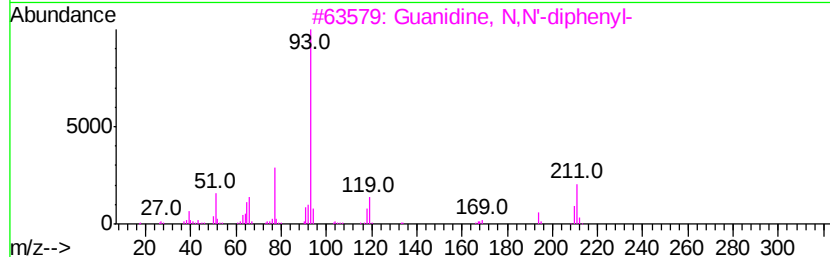
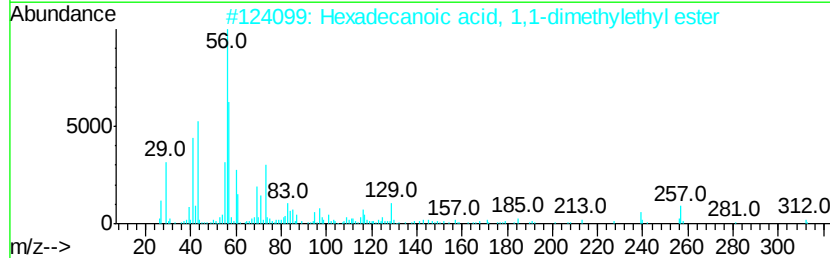
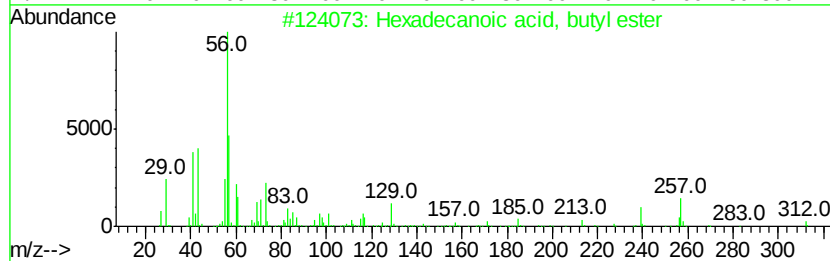
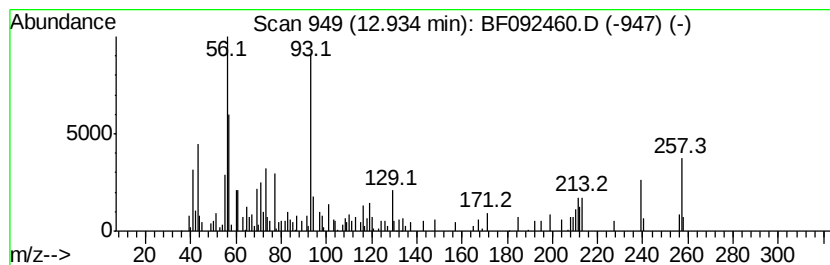
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown12.93 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.93	2.62 ng	116425	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	46
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	37
3		Guanidine, N,N'-diphenyl-	211	C13H13N3	000102-06-7	20
4		Urea, N,N'-diphenyl-	212	C13H12N2O	000102-07-8	14
5		Propanamide, N-phenyl-3-(phenylt...	257	C15H15NOS	126400-65-5	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092460.D
Acq On : 25 Jan 2017 5:37
Operator : UM/SJ
Sample : I1397-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-27

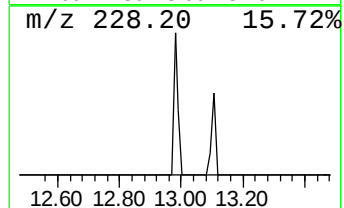
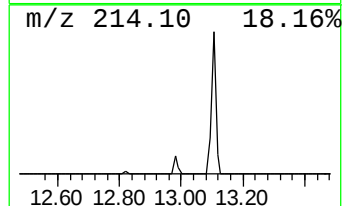
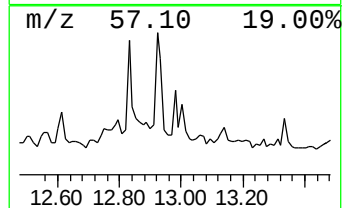
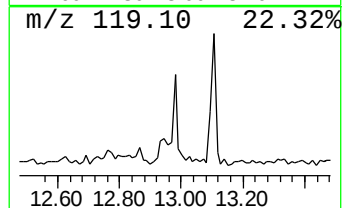
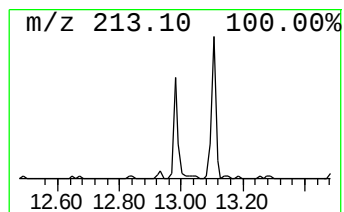
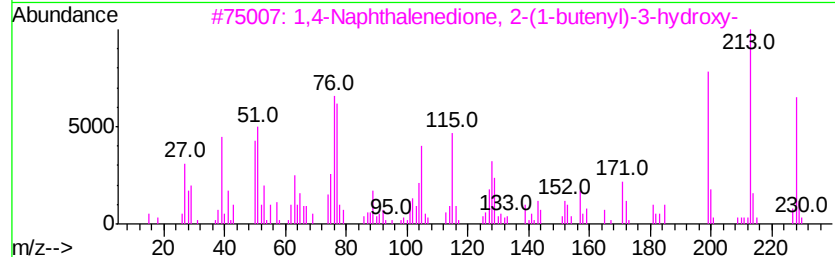
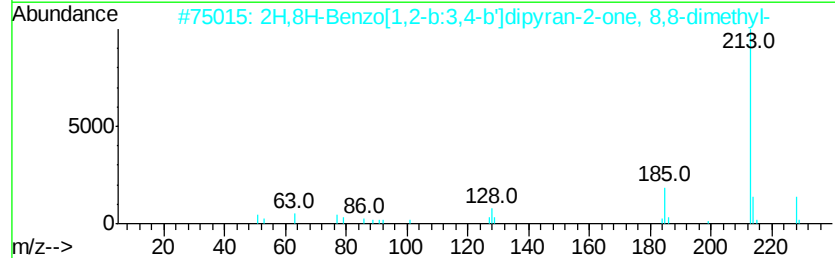
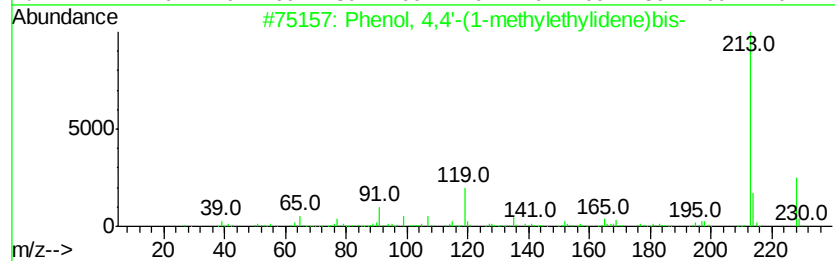
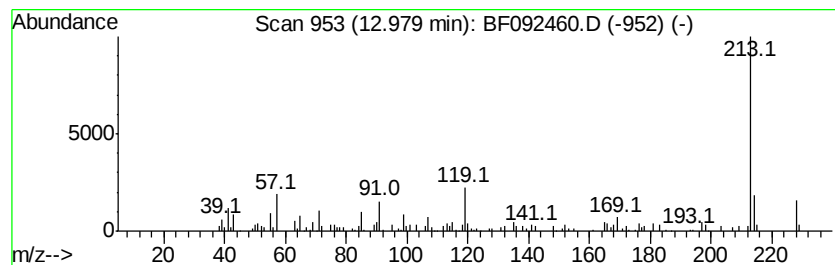
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 4,4'-(1-methylethyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.98	2.06 ng	91458	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	93
2		2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	52
3		1,4-Naphthalenedione, 2-(1-buten...	228	C14H12O3	029366-43-6	47
4		Trimethyl[5-(trimethylsilyl)-2-t...	228	C10H20SSi2	017906-71-7	42
5		2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
Data File : BF092460.D
Acq On : 25 Jan 2017 5:37
Operator : UM/SJ
Sample : I1397-06
Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-27

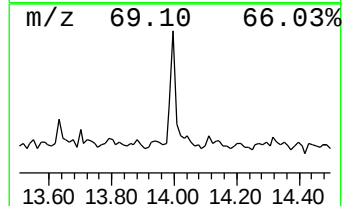
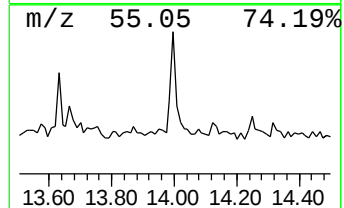
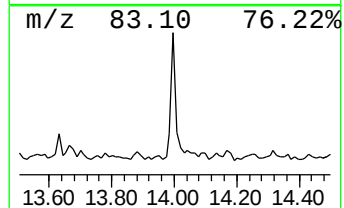
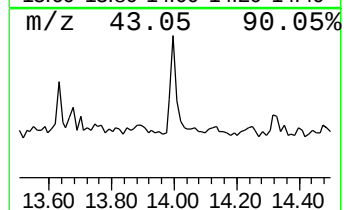
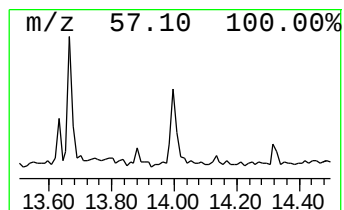
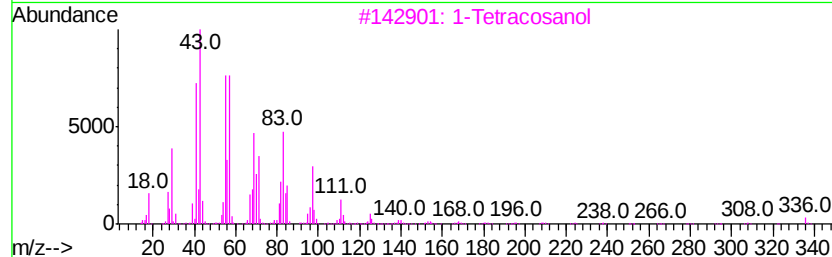
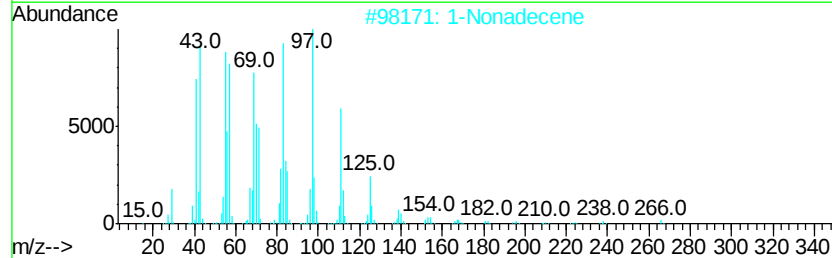
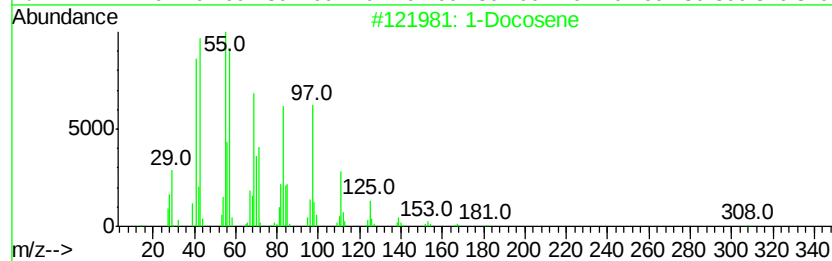
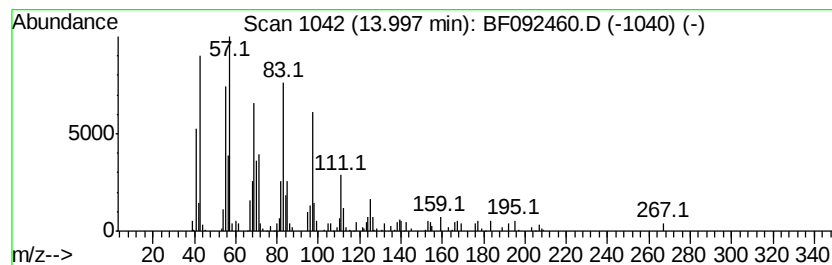
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	2.78 ng	123273	Chrysene-d12	14.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	94
2	1-Nonadecene		266	C19H38	018435-45-5	91
3	1-Tetracosanol		354	C24H50O	000506-51-4	91
4	Dichloroacetic acid, heptadecyl ...		366	C19H36Cl2O2	1000282-98-2	91
5	2- Chloropropionic acid, pentade...		318	C18H35ClO2	1000292-44-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012417\
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Misc :
ALS Vial : 41 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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...	5.14	13.1 ng		619668	1	6.97	949595	20.0
unknown6.73	6.73	70.2 ng		3330890	1	6.97	949595	20.0
Benzenesulfonamid...	11.40	2.4 ng		145899	4	11.52	1224900	20.0
Dodecanoic acid	12.04	3.1 ng		189258	4	11.52	1224900	20.0
unknown12.93	12.93	2.6 ng		116425	5	14.15	887143	20.0
Phenol, 4,4'-(1-m...	12.98	2.1 ng		91458	5	14.15	887143	20.0
1-Docosene	14.00	2.8 ng		123273	5	14.15	887143	20.0