

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
 Data File : BF086223.D
 Acq On : 15 Apr 2016 18:22
 Operator : UM/SJ
 Sample : H2531-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DSN001

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-BF041516.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	2.155	4	6	23	rVB3	97924	330066	4.19%	0.533%
2	5.070	259	261	266	rBV	97956	142960	1.82%	0.231%
3	5.481	294	297	299	rBV	3958582	3691467	46.87%	5.967%
4	6.510	384	387	389	rBV	2876089	2659245	33.77%	4.298%
5	6.659	397	400	402	rBV	5676501	6176269	78.42%	9.983%
6	6.887	418	420	423	rBV	1499794	1733635	22.01%	2.802%
7	7.047	431	434	437	rVB	5104191	5314841	67.48%	8.590%
8	7.459	467	470	472	rBV	4793205	5280129	67.04%	8.534%
9	8.179	530	533	535	rBV	2740945	2404845	30.53%	3.887%
10	9.253	624	627	630	rBV	5417742	7875741	100.00%	12.730%
11	9.642	660	661	664	rBV	303409	442970	5.62%	0.716%
12	9.870	679	681	683	rVB	307405	239116	3.04%	0.386%
13	9.928	684	686	689	rVB	2143841	2475760	31.44%	4.002%
14	10.099	699	701	703	rBV2	57145	103807	1.32%	0.168%
15	10.373	721	725	726	rBV2	410645	437726	5.56%	0.708%
16	10.591	741	744	747	rBV	140292	244784	3.11%	0.396%
17	10.716	752	755	758	rVV	3469316	4203983	53.38%	6.795%
18	10.842	764	766	771	rVB2	490154	552832	7.02%	0.894%
19	11.036	781	783	785	rBV	57352	81639	1.04%	0.132%
20	11.288	803	805	807	rBV	270710	254915	3.24%	0.412%
21	11.413	814	816	818	rVV	2840027	2398193	30.45%	3.876%
22	11.951	860	863	864	rBV	412252	489764	6.22%	0.792%
23	11.973	864	865	867	rVB2	103712	137815	1.75%	0.223%
24	12.648	920	924	929	rBV4	51925	145255	1.84%	0.235%
25	12.728	929	931	938	rBV2	350212	641811	8.15%	1.037%
26	12.831	938	940	942	rBV2	134464	116336	1.48%	0.188%
27	12.888	942	945	948	rVB2	98321	170751	2.17%	0.276%
28	13.002	952	955	958	rBV	4937938	6229603	79.10%	10.069%
29	13.242	972	976	978	rBV	195820	237453	3.01%	0.384%
30	13.539	1000	1002	1004	rBV	78500	117935	1.50%	0.191%
31	13.585	1004	1006	1007	rVV	226412	204729	2.60%	0.331%
32	13.905	1031	1034	1039	rBV	728699	1180752	14.99%	1.908%
33	14.042	1044	1046	1049	rBV	1716590	1888245	23.98%	3.052%
34	14.225	1060	1062	1070	rVB	488156	500213	6.35%	0.809%

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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	14.534	1087	1089	1093	rBV	481734	509106	6.46%	0.823%
36	14.831	1113	1115	1119	rBV	253607	315206	4.00%	0.509%
37	14.911	1119	1122	1124	rVB	74075	87195	1.11%	0.141%
38	15.162	1142	1144	1150	rBV	148534	207186	2.63%	0.335%
39	15.482	1169	1172	1175	rBV	1025609	1310114	16.63%	2.118%
40	15.540	1175	1177	1184	rVB	73224	144654	1.84%	0.234%
41	17.483	1342	1347	1353	rBV	71202	190191	2.41%	0.307%

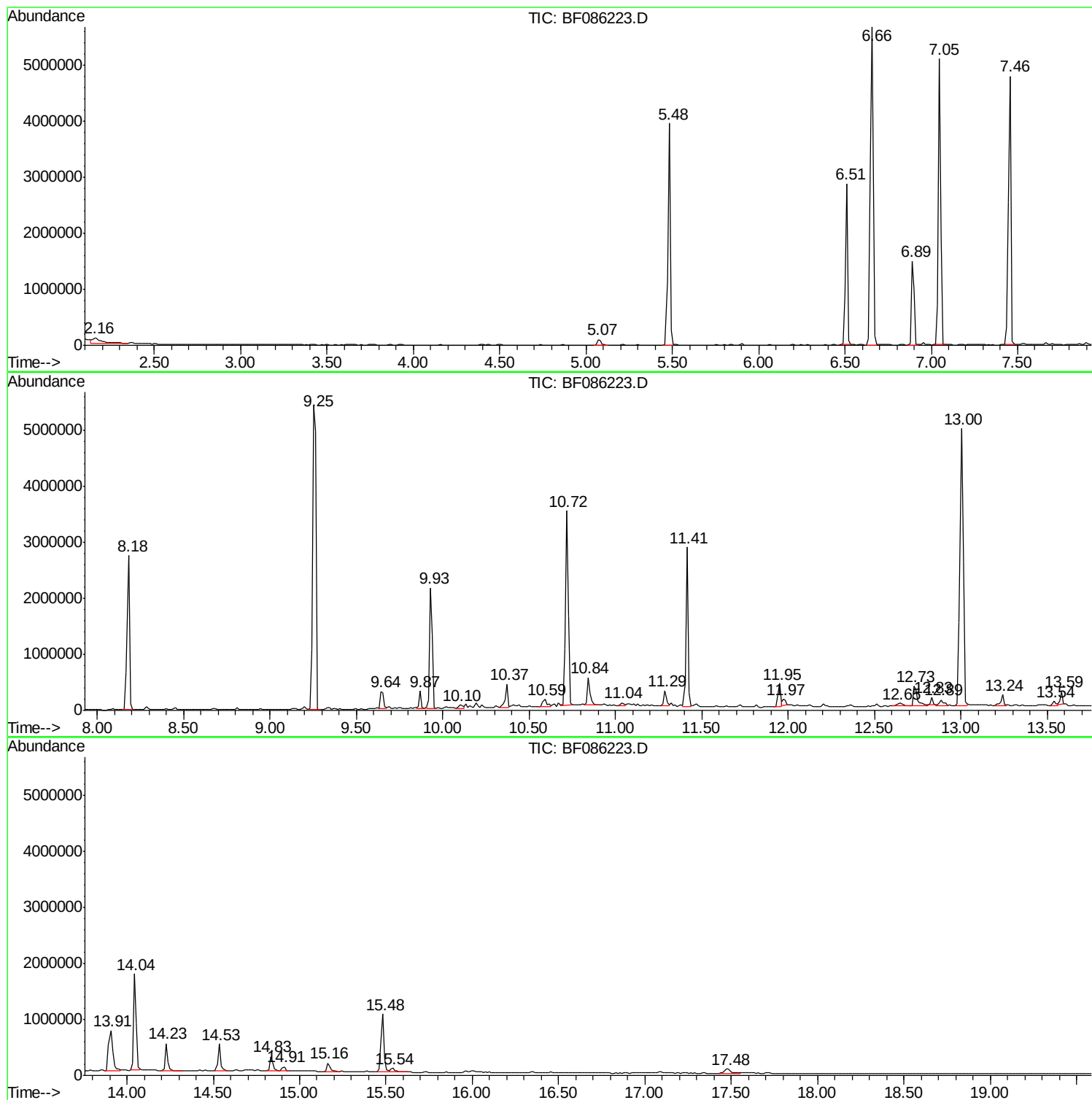
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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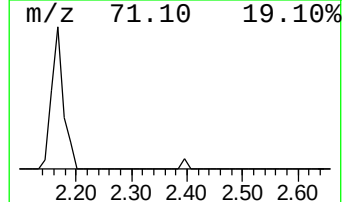
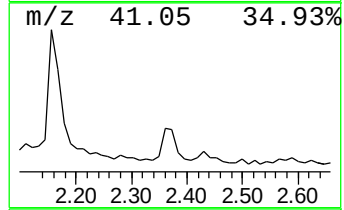
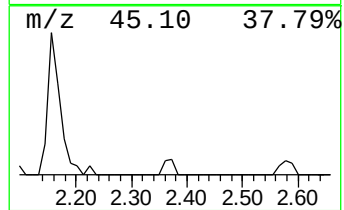
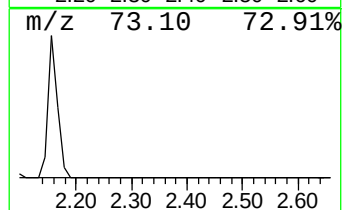
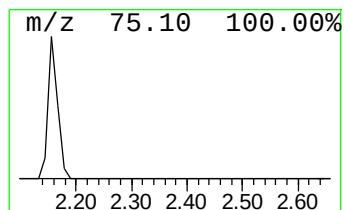
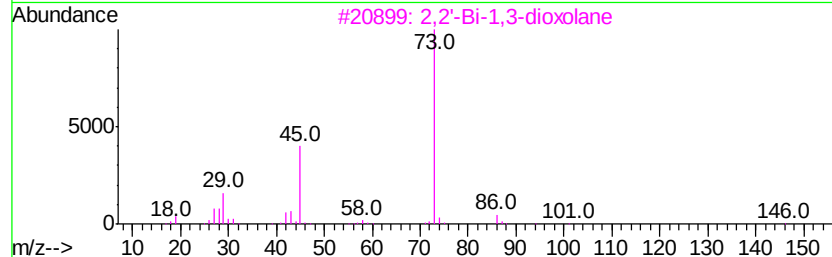
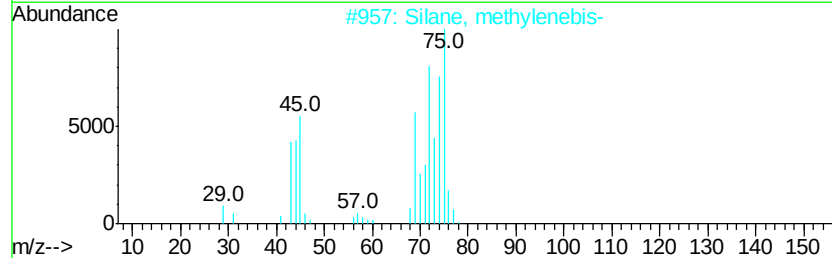
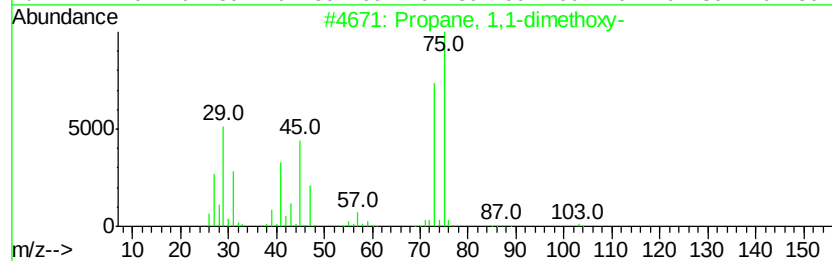
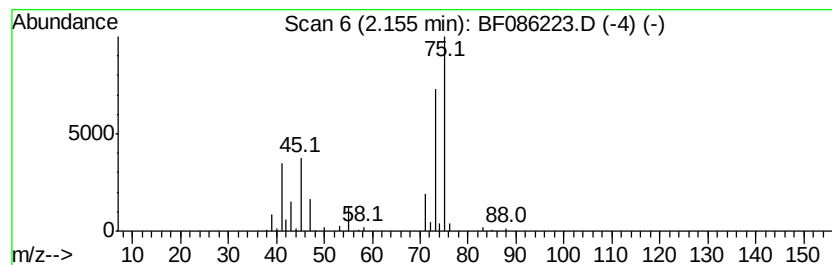
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	3.81 ng	330066	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	50
2		Silane, methylenebis-	76	CH8Si2	001759-88-2	9
3		2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9
4		Chloromethyl cyanide	75	C2H2ClN	000107-14-2	5
5		Glycine	75	C2H5NO2	000056-40-6	5



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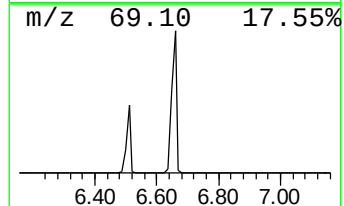
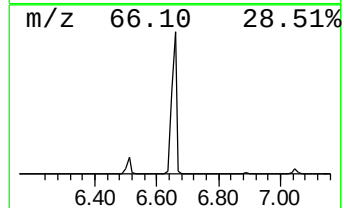
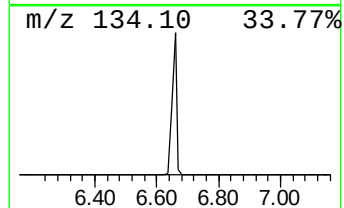
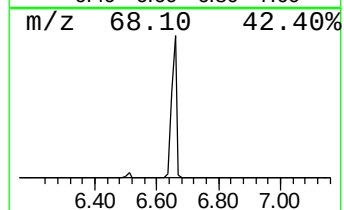
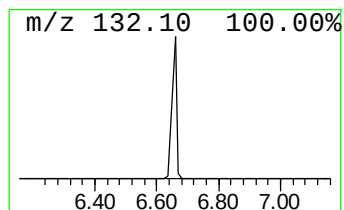
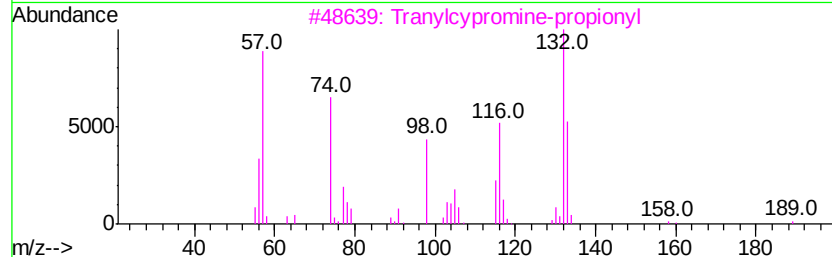
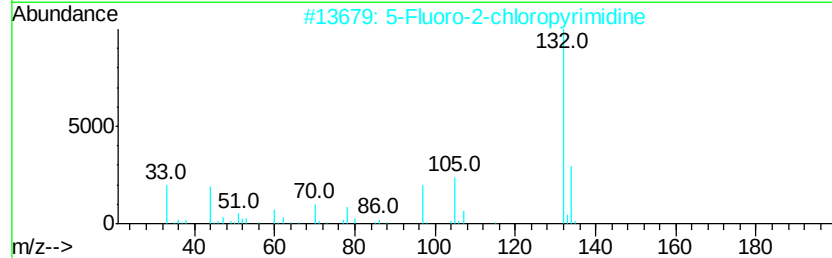
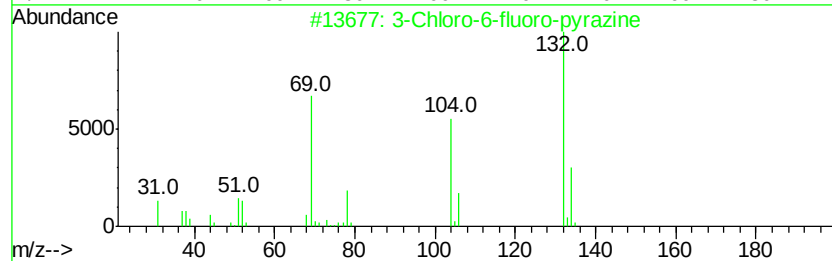
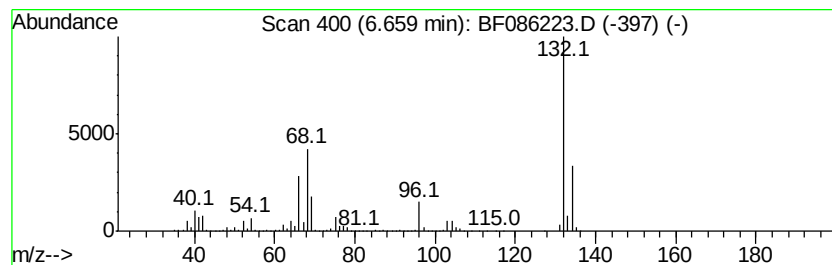
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	71.25 ng	6176270	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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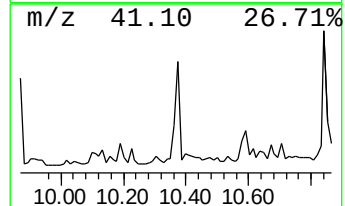
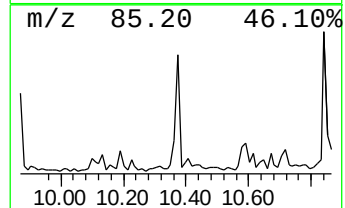
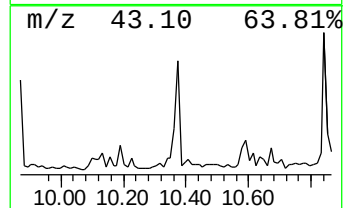
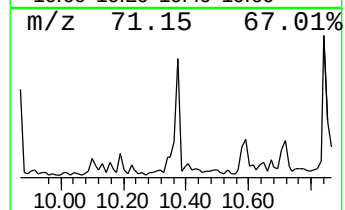
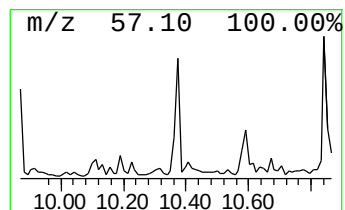
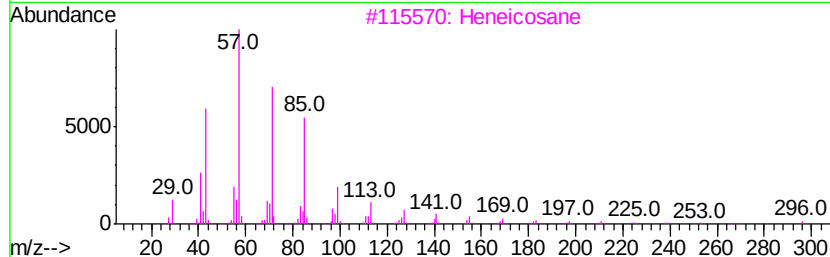
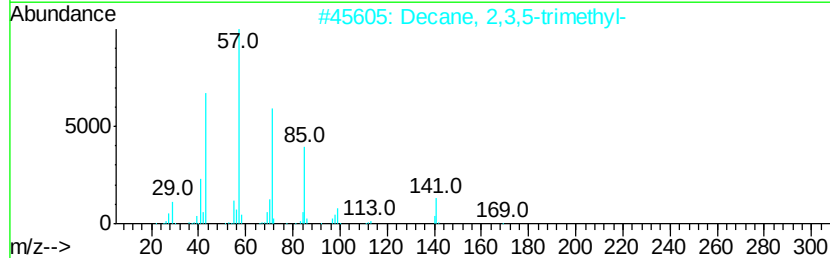
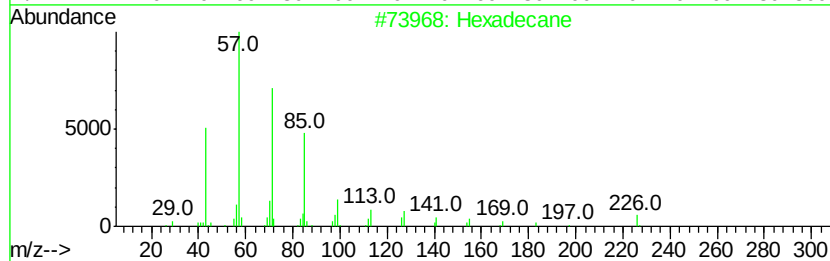
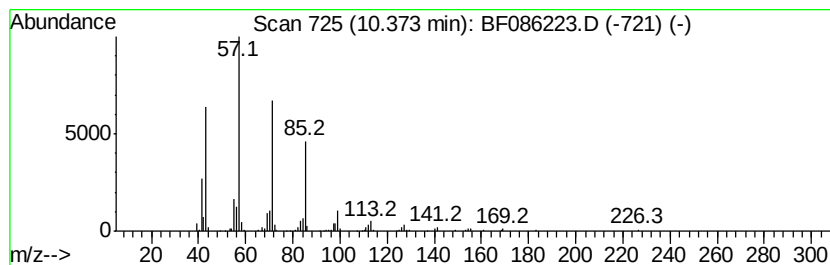
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.37	3.54 ng	437726	Acenaphthene-d10		9.93
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tridecane	184	C13H28	000629-50-5	90
5	Tetradecane	198	C14H30	000629-59-4	87



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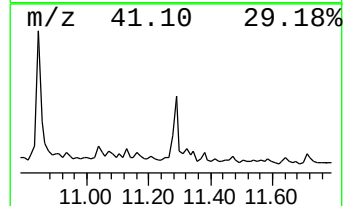
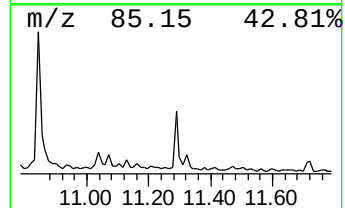
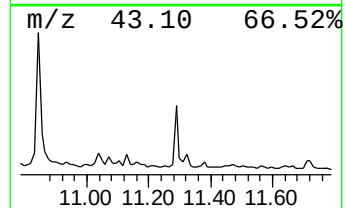
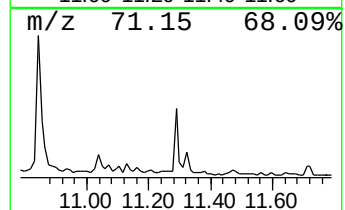
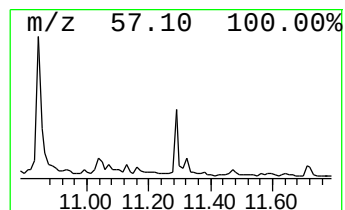
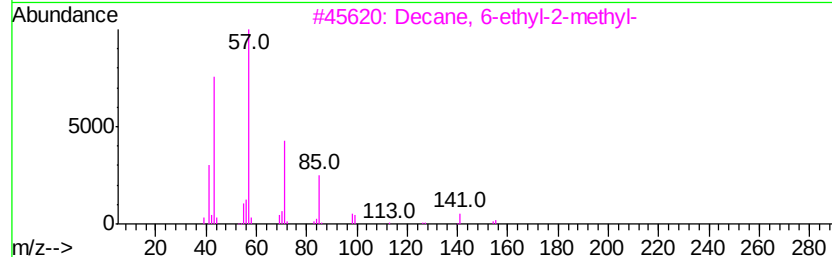
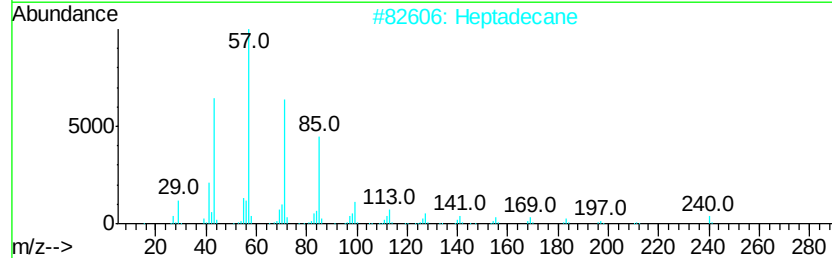
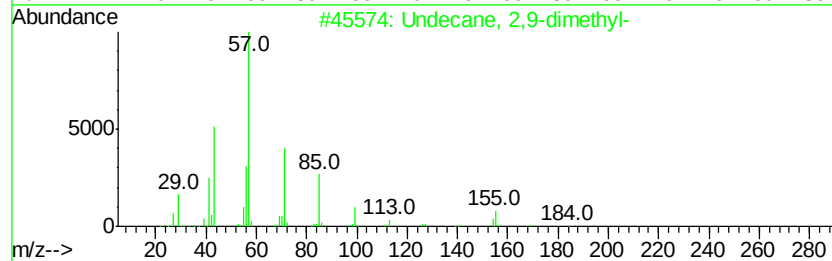
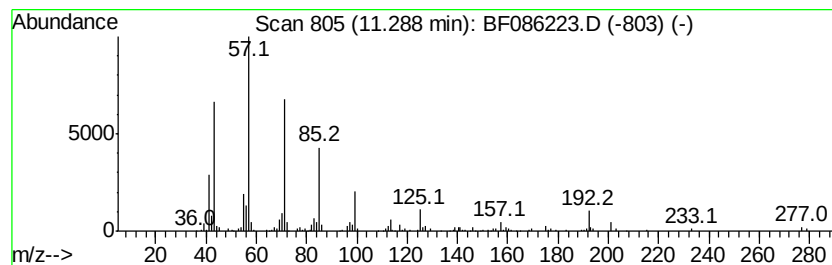
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecane, 2,9-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.29	2.13 ng	254915	Phenanthrene-d10		11.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,9-dimethyl-	184	C13H28	017301-26-7	59
2			Heptadecane	240	C17H36	000629-78-7	50
3			Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	50
4			Hexadecane	226	C16H34	000544-76-3	43
5			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	43



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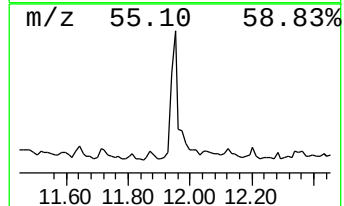
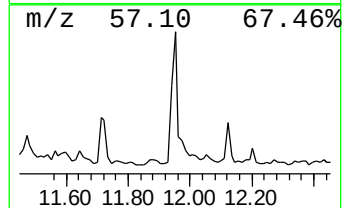
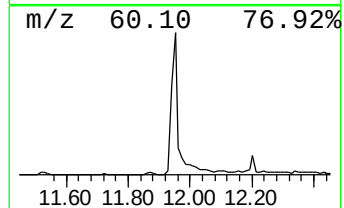
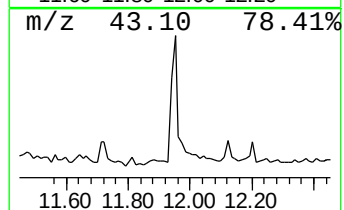
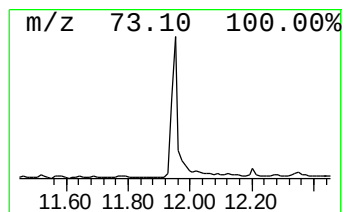
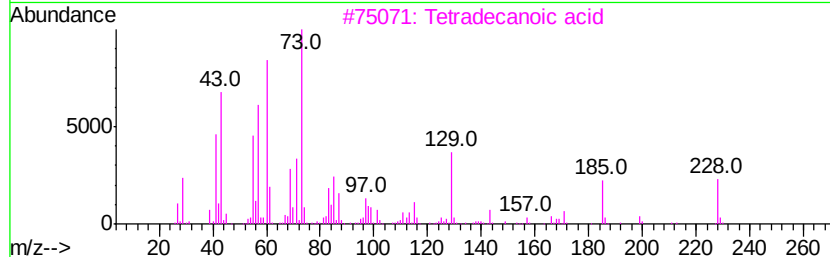
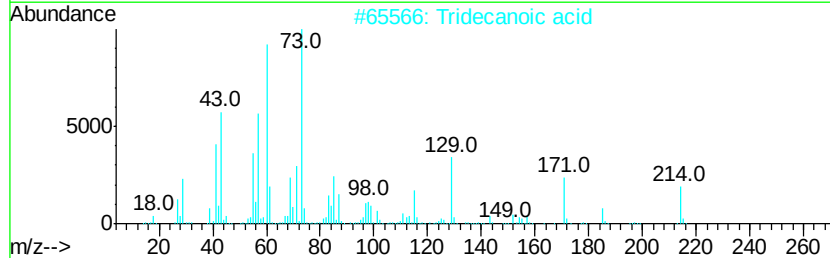
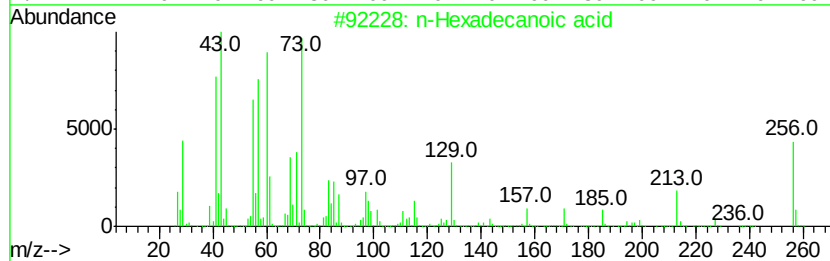
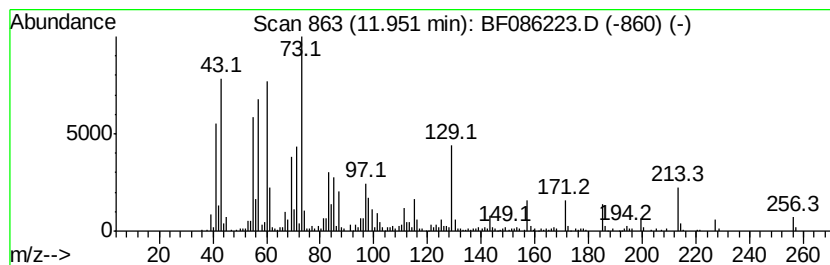
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.95	4.08 ng	489764	Phenanthrene-d10	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	74
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72



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Misc :
ALS Vial : 6 Sample Multiplier: 1

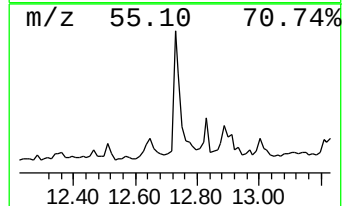
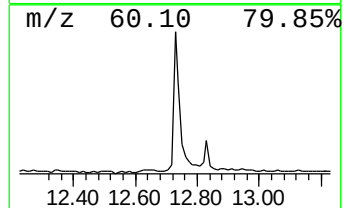
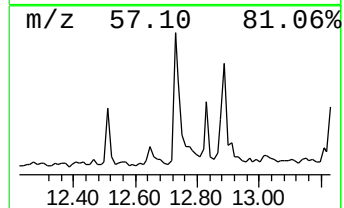
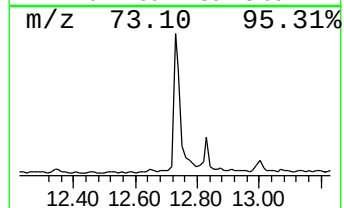
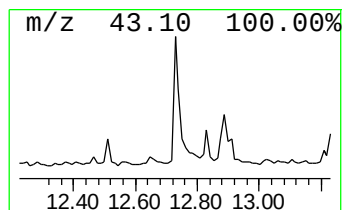
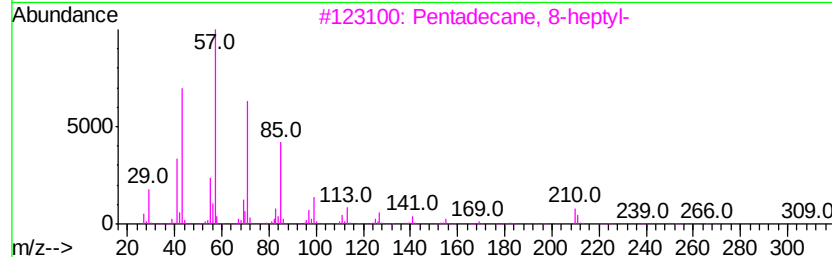
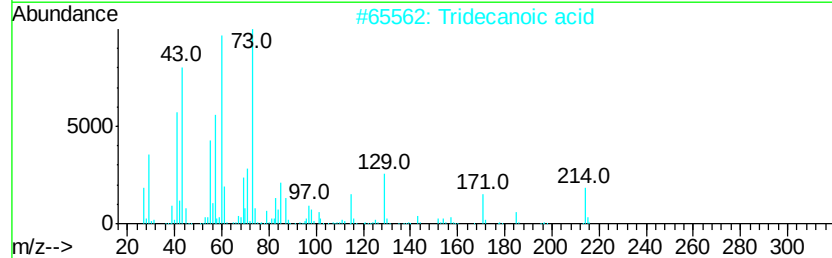
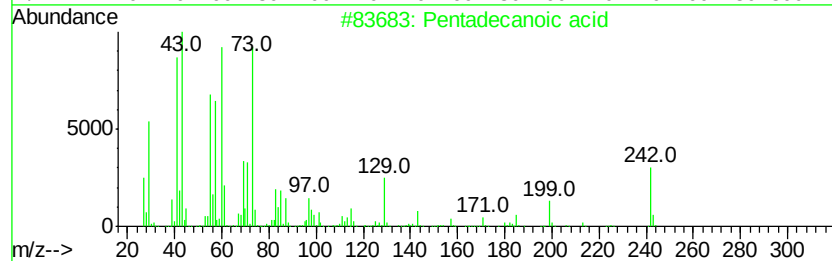
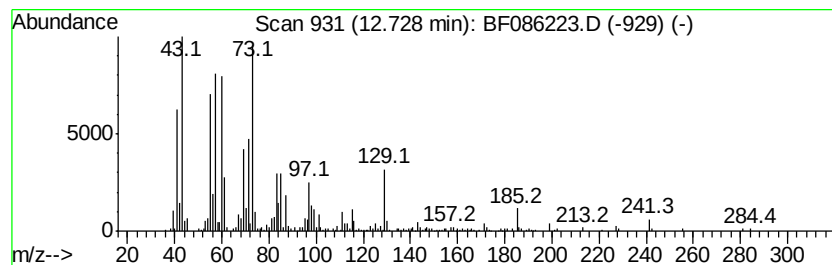
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown12.73 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.73	5.35 ng	641811	Phenanthrene-d10		11.41
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	43
2	Tridecanoic acid	214	C13H26O2	000638-53-9	35
3	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	14
4	Dodecane, 1,2-dibromo-	326	C12H24Br2	055334-42-4	14
5	Dotriacontane	451	C32H66	000544-85-4	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
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Acq On : 15 Apr 2016 18:22
Operator : UM/SJ
Sample : H2531-01
Misc :
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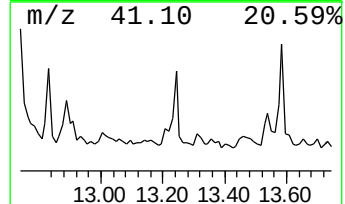
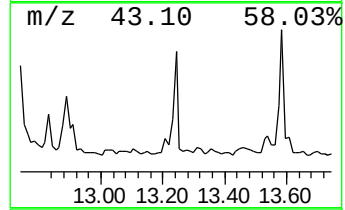
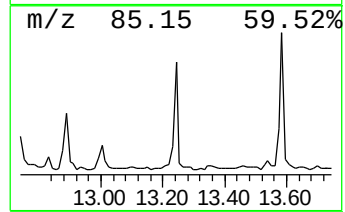
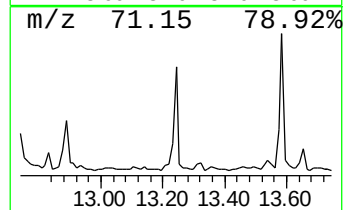
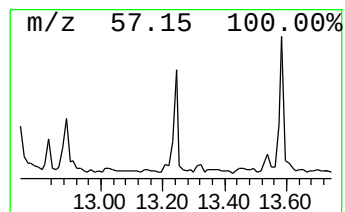
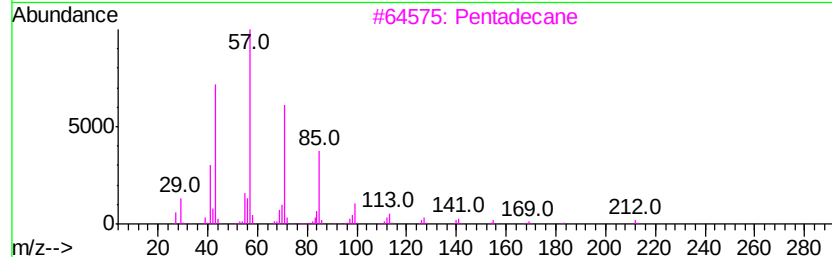
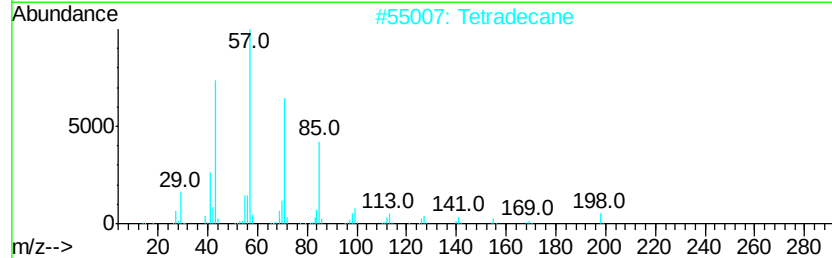
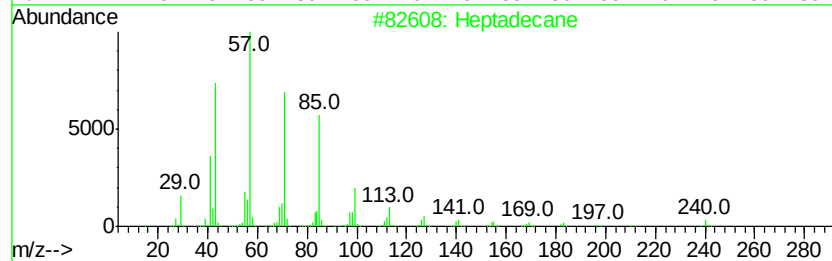
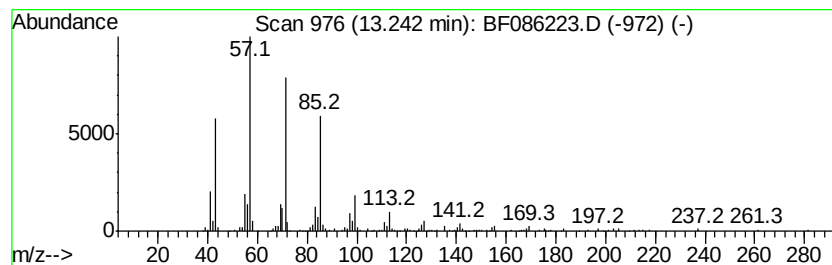
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.24	2.52 ng	237453	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Tetradecane	198	C14H30	000629-59-4	86
3	Pentadecane	212	C15H32	000629-62-9	72
4	Eicosane	282	C20H42	000112-95-8	72
5	Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
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Sample : H2531-01
Misc :
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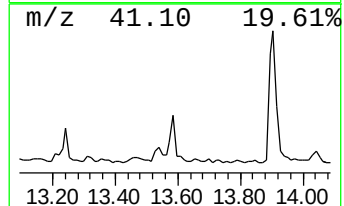
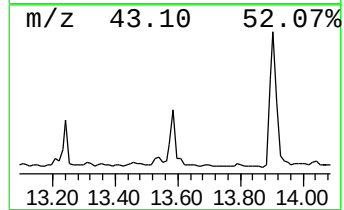
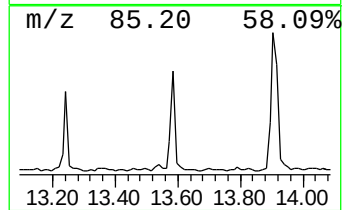
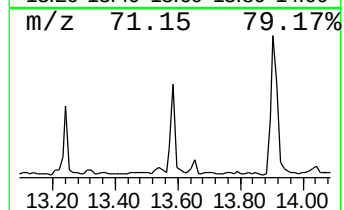
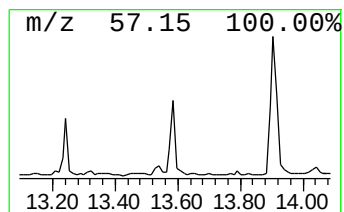
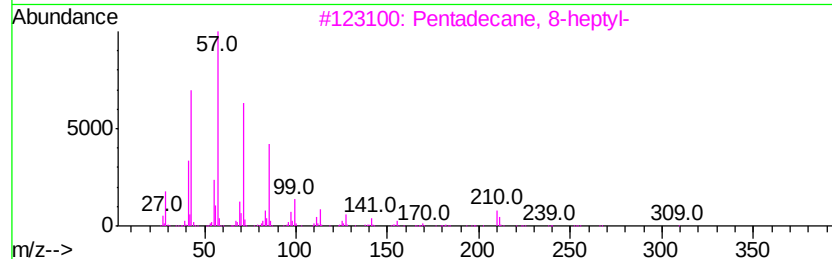
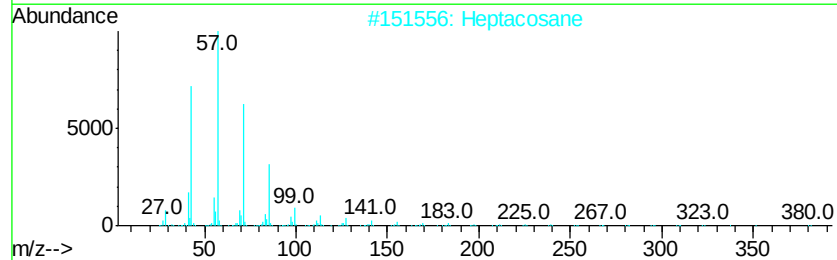
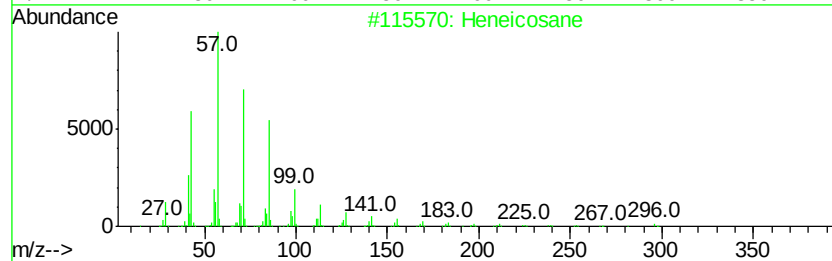
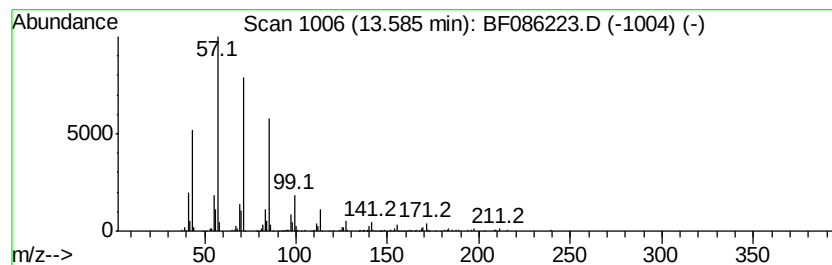
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	2.17 ng	204729	Chrysene-d12	14.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	91
2	Heptacosane	380 C27H56	000593-49-7	83
3	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	72
4	Hexadecane	226 C16H34	000544-76-3	72
5	Octadecane	254 C18H38	000593-45-3	72



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086223.D
Acq On : 15 Apr 2016 18:22
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Sample : H2531-01
Misc :
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Instrument :
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ClientSampleId :
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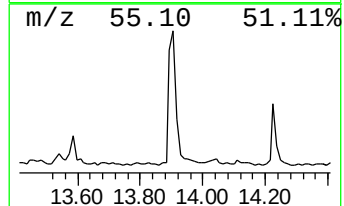
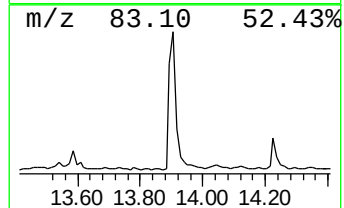
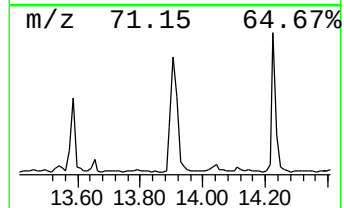
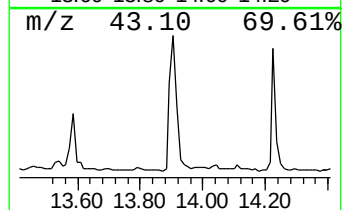
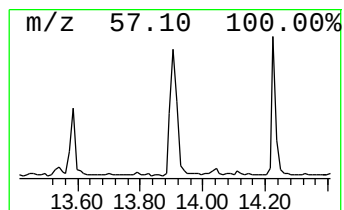
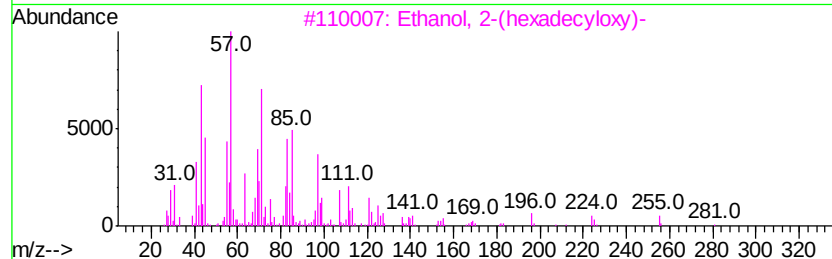
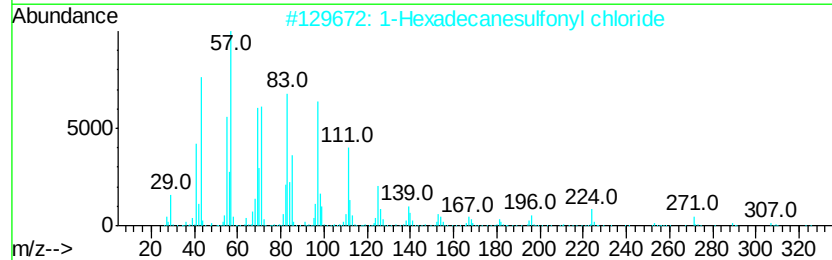
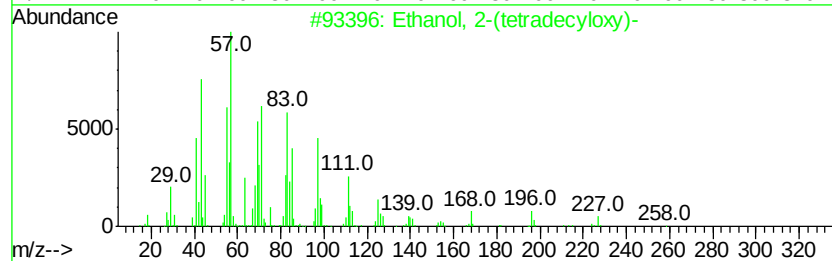
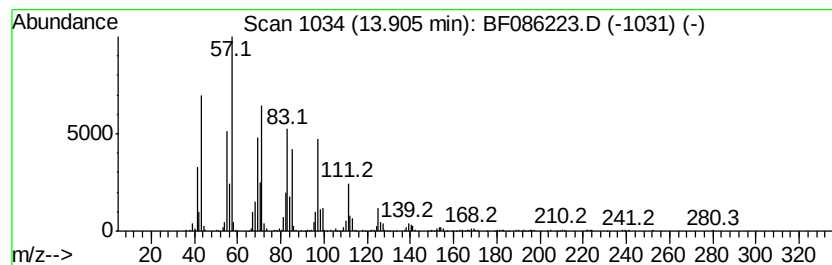
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethanol, 2-(tetradecyloxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.91	12.51 ng	1180750	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	90
3		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	80
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	76
5		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	74



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
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Acq On : 15 Apr 2016 18:22
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Misc :
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ClientSampleId :
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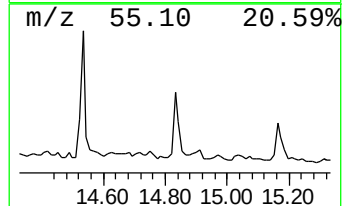
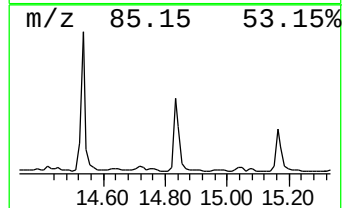
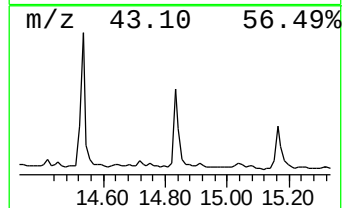
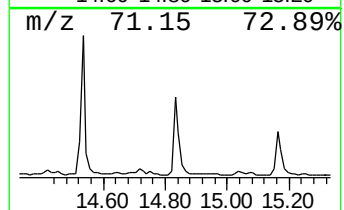
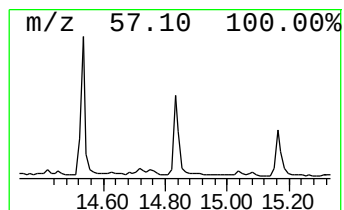
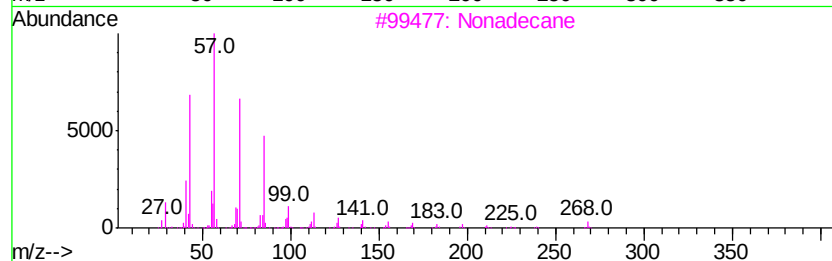
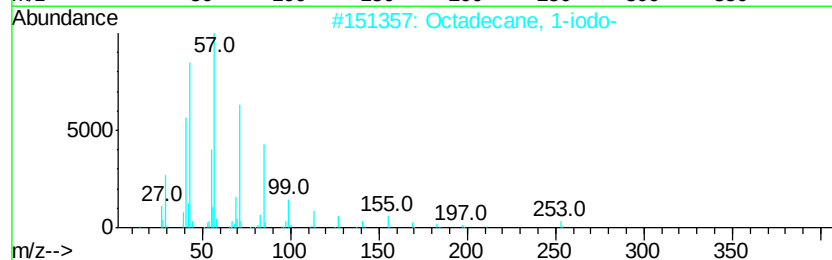
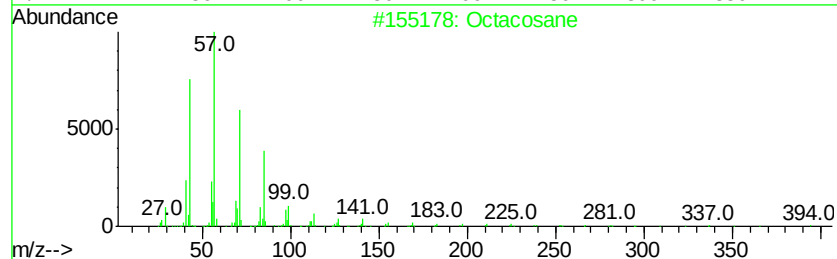
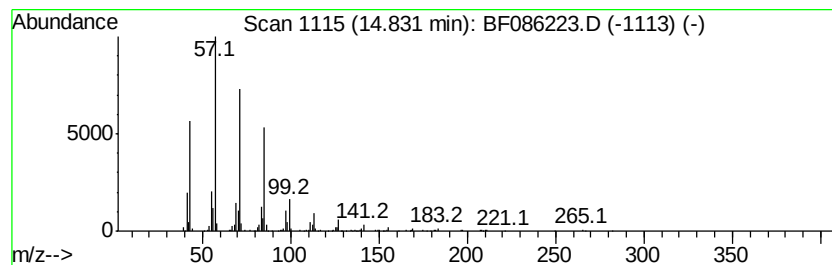
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	4.81 ng	315206	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	87
2		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3		Nonadecane	268	C19H40	000629-92-5	86
4		Tetracosane	338	C24H50	000646-31-1	86
5		Pentadecane	212	C15H32	000629-62-9	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086223.D
Acq On : 15 Apr 2016 18:22
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Sample : H2531-01
Misc :
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Instrument :
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ClientSampleId :
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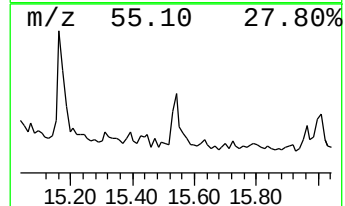
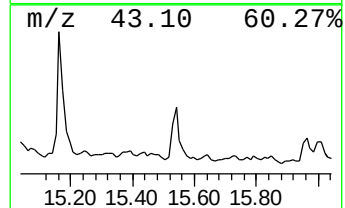
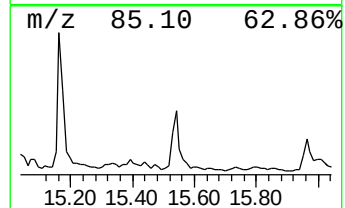
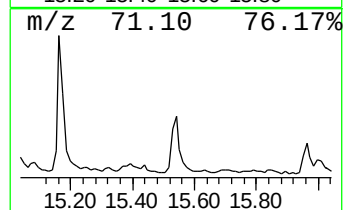
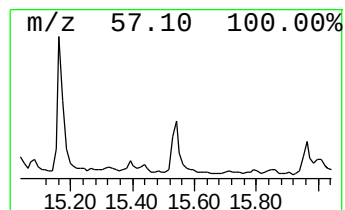
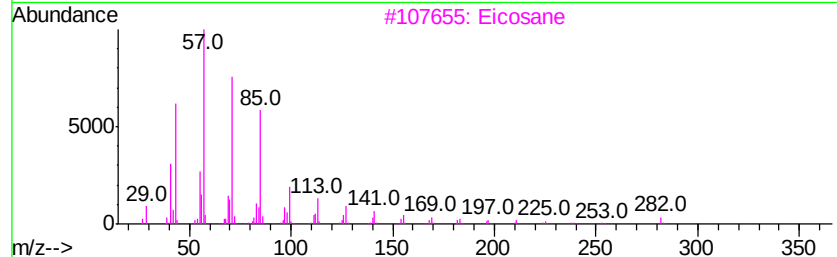
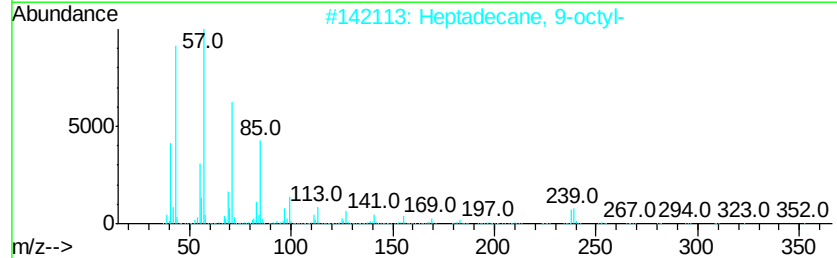
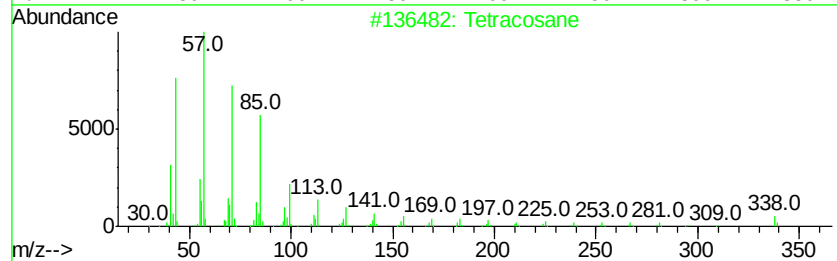
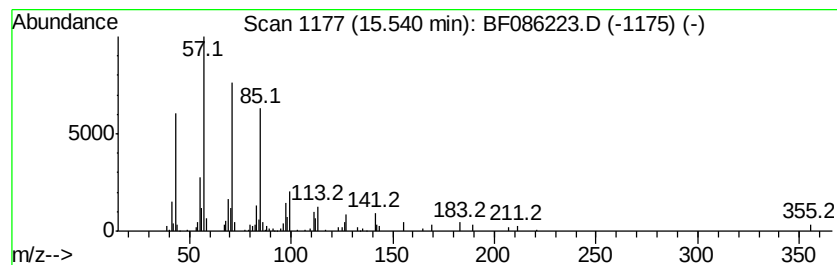
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Tetracosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	2.21 ng	144654	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
3		Eicosane	282	C20H42	000112-95-8	87
4		Triacontane	422	C30H62	000638-68-6	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041516\
Data File : BF086223.D
Acq On : 15 Apr 2016 18:22
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Sample : H2531-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

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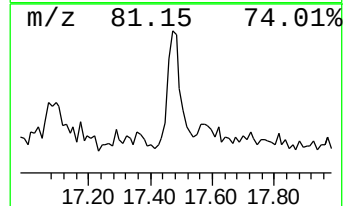
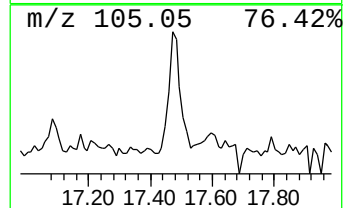
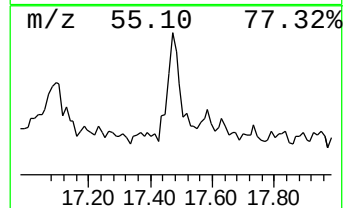
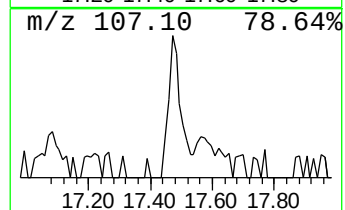
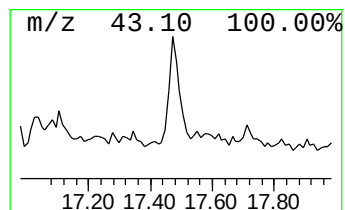
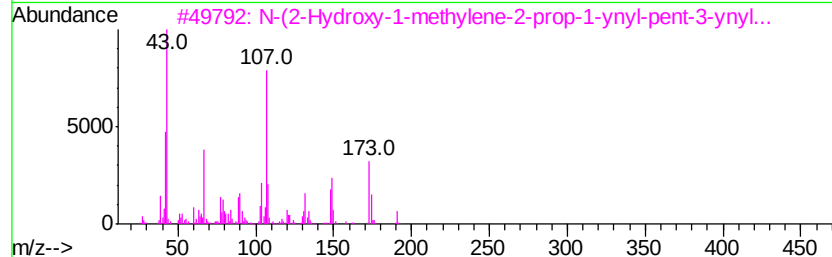
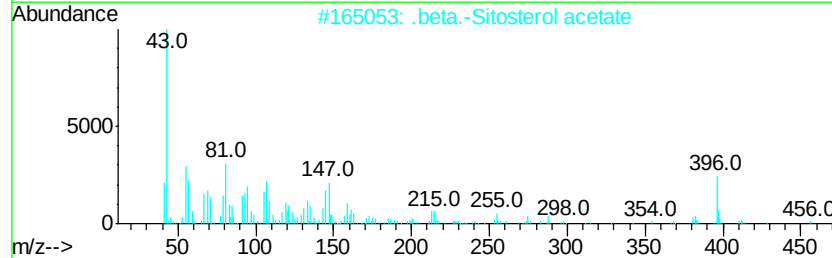
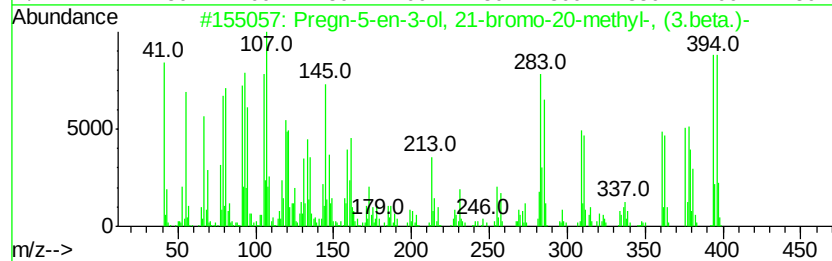
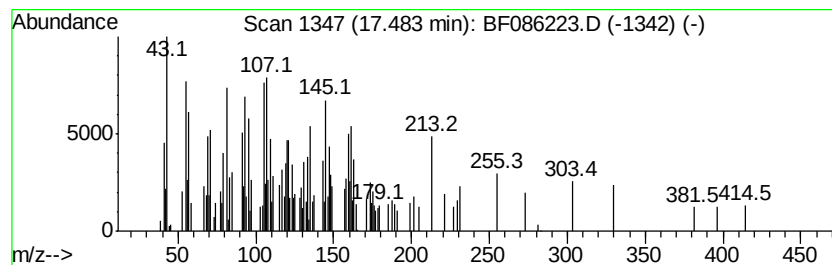
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown17.48 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.48	2.90 ng	190191	Perylene-d12	15.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	35
2		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	27
3		N-(2-Hydroxy-1-methylene-2-prop-...	191	C11H13NO2	1000194-35-2	15
4		cis-4-Acetoxy-trans-1-(m-methoxy...	273	C16H19NO3	1000241-10-4	14
5		3-Methoxy-N-[3-(4-nitro-phenylam...	329	C17H19N3O4	1000297-02-0	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041516\
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Acq On : 15 Apr 2016 18:22
Operator : UM/SJ
Sample : H2531-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DSN001

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041516.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
Propane, 1,1-dime...	2.16	3.8	ng	330066	1	6.89	1733640	20.0
unknown6.66	6.66	71.3	ng	6176270	1	6.89	1733640	20.0
Hexadecane	10.37	3.5	ng	437726	3	9.93	2475760	20.0
Undecane, 2,9-dim...	11.29	2.1	ng	254915	4	11.41	2398190	20.0
n-Hexadecanoic acid	11.95	4.1	ng	489764	4	11.41	2398190	20.0
unknown12.73	12.73	5.3	ng	641811	4	11.41	2398190	20.0
Heptadecane	13.24	2.5	ng	237453	5	14.04	1888250	20.0
Heneicosane	13.59	2.2	ng	204729	5	14.04	1888250	20.0
Ethanol, 2-(tetra...	13.91	12.5	ng	1180750	5	14.04	1888250	20.0
Octacosane	14.83	4.8	ng	315206	6	15.48	1310110	20.0
Tetracosane	15.54	2.2	ng	144654	6	15.48	1310110	20.0
unknown17.48	17.48	2.9	ng	190191	6	15.48	1310110	20.0