

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
 Data File : BF085509.D
 Acq On : 17 Mar 2016 23:41
 Operator : UM/SJ
 Sample : H1774-02
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-23-COMP

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-BF031516.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	5.076	242	244	255	rVB	53669	73062	2.10%	0.206%
2	5.270	259	261	264	rBV3	303896	930832	26.79%	2.625%
3	5.476	276	279	281	rBV	2959096	3102237	89.30%	8.747%
4	5.921	316	318	321	rBV4	45409	78058	2.25%	0.220%
5	6.504	366	369	372	rBV	2468955	3237928	93.21%	9.130%
6	6.550	372	373	377	rVB4	52707	69850	2.01%	0.197%
7	6.641	379	381	384	rVB	3119239	3196518	92.01%	9.013%
8	6.699	384	386	388	rBV3	43600	106969	3.08%	0.302%
9	6.870	400	401	403	rBV	773342	808793	23.28%	2.280%
10	6.904	403	404	407	rVB3	31536	47261	1.36%	0.133%
11	7.030	413	415	417	rVB	2731253	2474794	71.24%	6.978%
12	7.156	424	426	428	rVB3	129139	161319	4.64%	0.455%
13	7.384	443	446	448	rBV4	113096	340011	9.79%	0.959%
14	7.441	448	451	453	rVV	2271036	2435499	70.11%	6.867%
15	7.487	453	455	456	rVB2	34000	60596	1.74%	0.171%
16	7.956	494	496	499	rBV4	54922	94736	2.73%	0.267%
17	8.127	509	511	512	rBV2	56256	65185	1.88%	0.184%
18	8.162	512	514	516	rVB	1298312	1177225	33.89%	3.319%
19	8.207	516	518	521	rBV4	66028	150337	4.33%	0.424%
20	8.493	540	543	548	rVB7	108114	294888	8.49%	0.831%
21	8.847	572	574	575	rBV2	104347	154003	4.43%	0.434%
22	9.019	587	589	590	rBV2	78268	67695	1.95%	0.191%
23	9.122	594	598	600	rVV5	109165	300861	8.66%	0.848%
24	9.236	606	608	611	rBV	3016234	3473919	100.00%	9.795%
25	9.293	611	613	616	rVB4	36039	74254	2.14%	0.209%
26	9.636	640	643	645	rVB	451970	512576	14.75%	1.445%
27	9.853	660	662	665	rVB	79088	112940	3.25%	0.318%
28	9.910	665	667	670	rVV	851154	1166376	33.58%	3.289%
29	10.002	673	675	679	rVB5	61574	108707	3.13%	0.307%
30	10.253	693	697	698	rBV4	100146	234921	6.76%	0.662%
31	10.299	698	701	702	rBV3	127465	306372	8.82%	0.864%
32	10.562	721	724	728	rBV	42264	85527	2.46%	0.241%
33	10.699	734	736	739	rBV2	1524505	2227653	64.13%	6.281%
34	10.825	745	747	753	rVB	104711	181746	5.23%	0.512%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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35	11.019	761	764	768	rBV3	15110	40380	1.16%	0.114%
36	11.270	784	786	787	rBV	73078	71104	2.05%	0.200%
37	11.396	795	797	800	rBV	1216759	1140545	32.83%	3.216%
38	11.465	800	803	805	rVB2	18714	36707	1.06%	0.103%
39	11.933	841	844	846	rBV	354399	455662	13.12%	1.285%
40	12.608	900	903	905	rBV	57598	68736	1.98%	0.194%
41	12.711	910	912	918	rBV	184827	204404	5.88%	0.576%
42	12.802	918	920	922	rBV	106612	110699	3.19%	0.312%
43	12.985	933	936	938	rBV	3195084	2978246	85.73%	8.397%
44	13.511	980	982	983	rBV	82246	70244	2.02%	0.198%
45	13.876	1011	1014	1021	rBV	319518	375378	10.81%	1.058%
46	14.036	1024	1028	1030	rBV	697885	938970	27.03%	2.648%
47	14.505	1067	1069	1075	rVB2	30526	48495	1.40%	0.137%
48	15.054	1115	1117	1121	rBV	26907	59574	1.71%	0.168%
49	15.134	1122	1124	1128	rVB2	21367	37103	1.07%	0.105%
50	15.465	1150	1153	1156	rBV	597577	781764	22.50%	2.204%
51	15.968	1195	1197	1204	rVB3	35227	70842	2.04%	0.200%
52	16.414	1232	1236	1242	rBV2	17611	63745	1.83%	0.180%

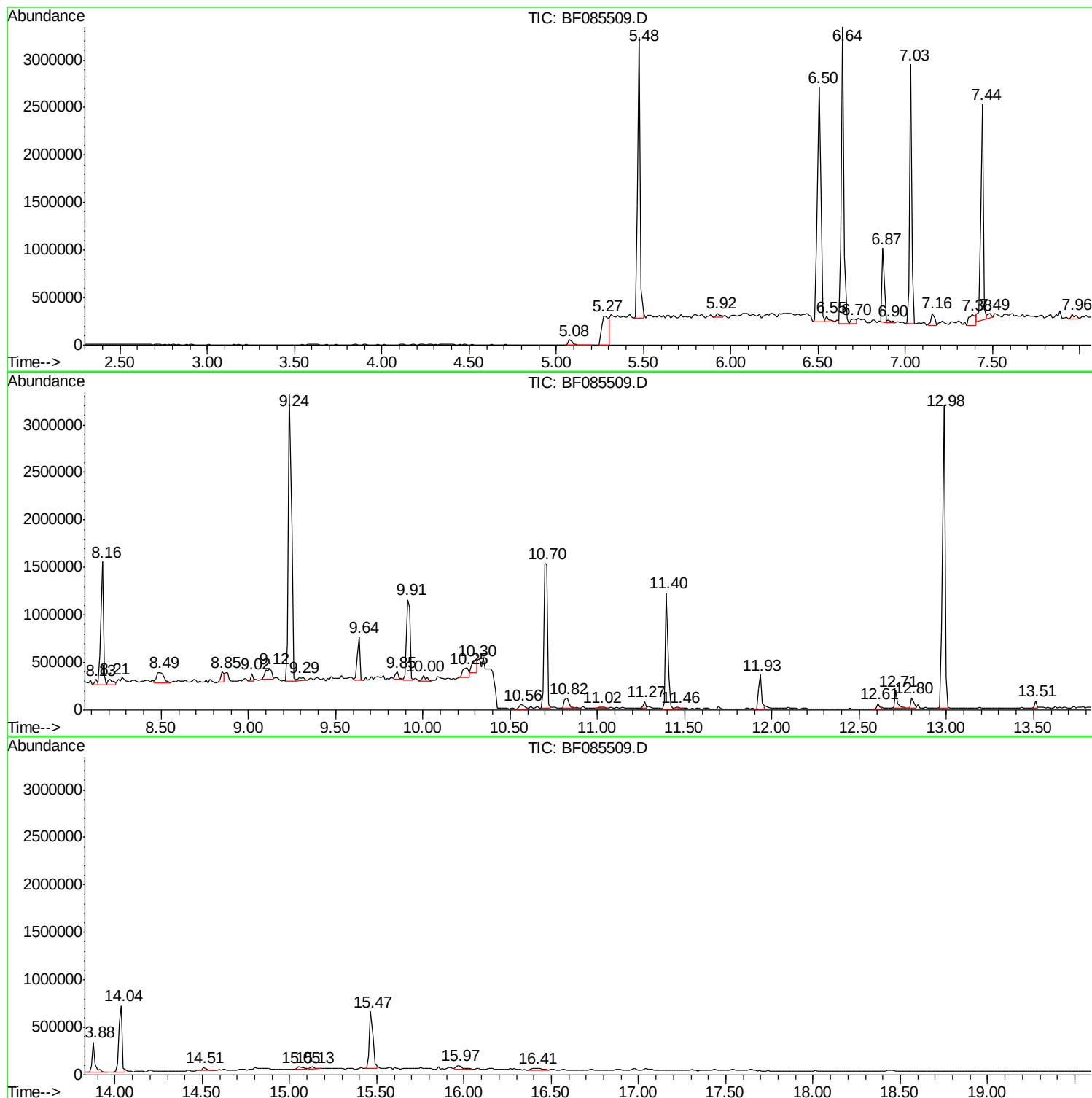
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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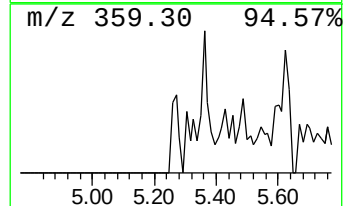
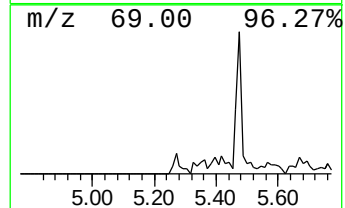
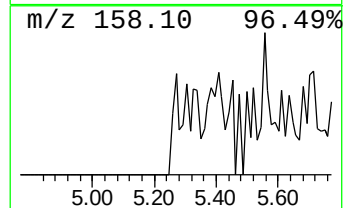
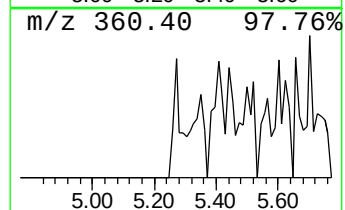
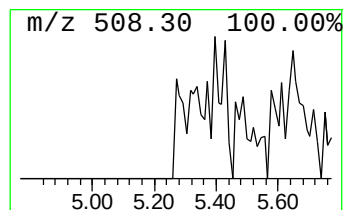
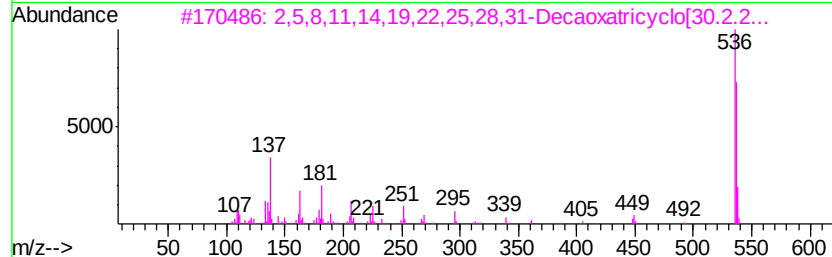
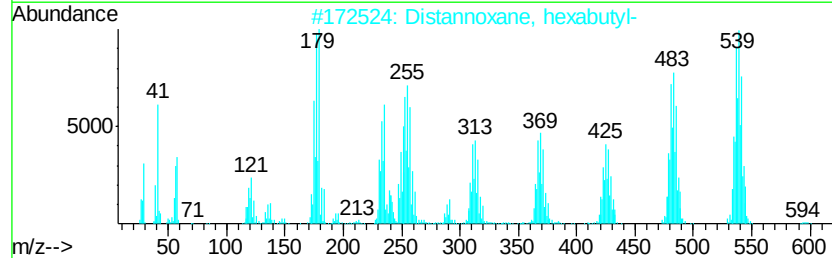
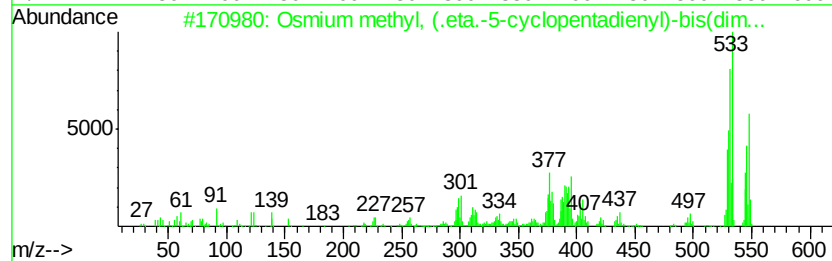
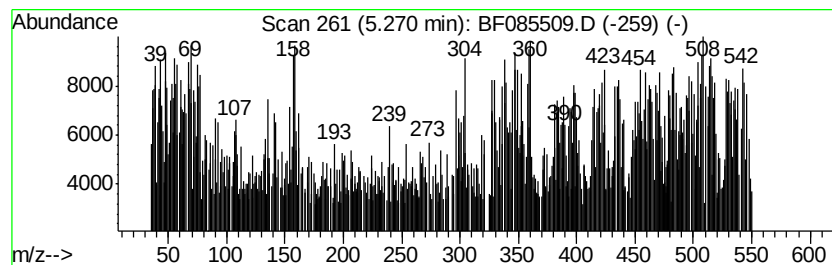
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.27 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	23.02 ng	930832	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Osmium methyl, (.eta.-5-cyclopentadienyl)-bis(dimethylamino)phosphine	548	C22H30Osp2	1000158-92-4	25
2		Distannoxane, hexabutyl-	598	C24H54OSn2	000056-35-9	12
3		2,5,8,11,14,19,22,25,28,31-Decaoxatricyclo[30.2.2.0]	536	C28H40O10	053914-95-7	11
4		Heptamethylethyl octasilsesquioxane	550	C9H26O12Si8	077626-17-6	10
5		5-Methyl-4-triphenylsilyl-2-(1-benzyl-1-phenylethyl)-1,3-dioxane	531	C32H26BrNSi	037965-29-0	10



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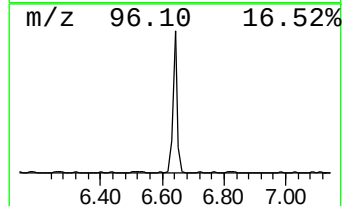
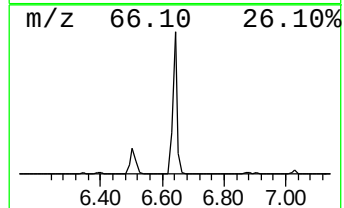
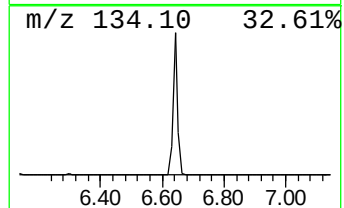
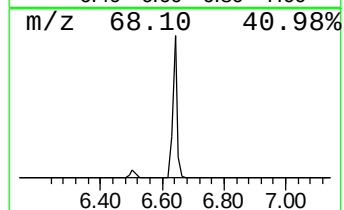
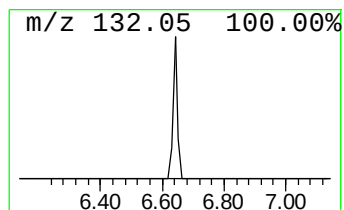
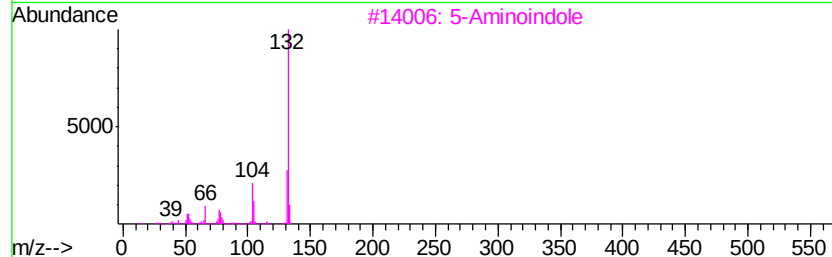
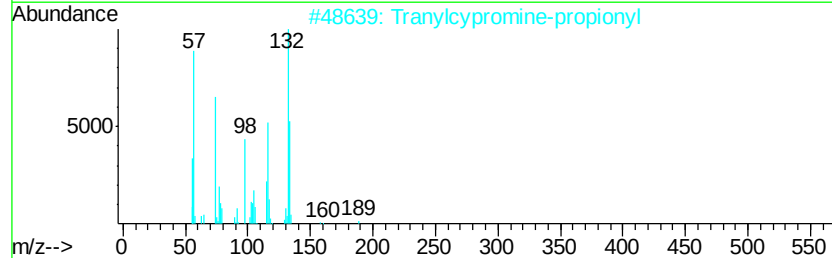
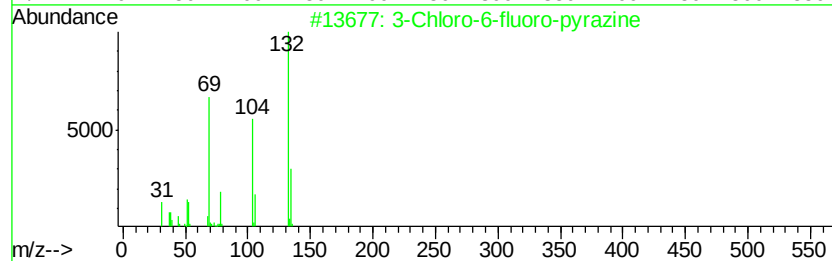
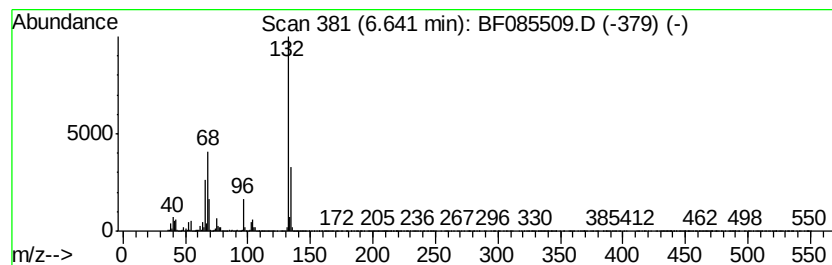
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	79.04 ng	3196520	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	9
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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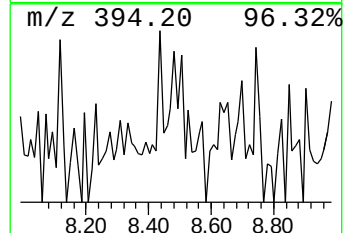
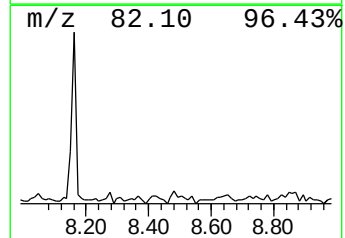
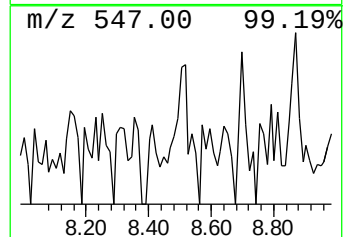
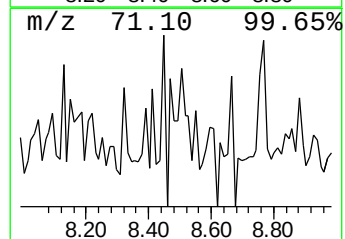
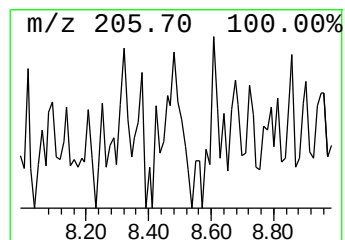
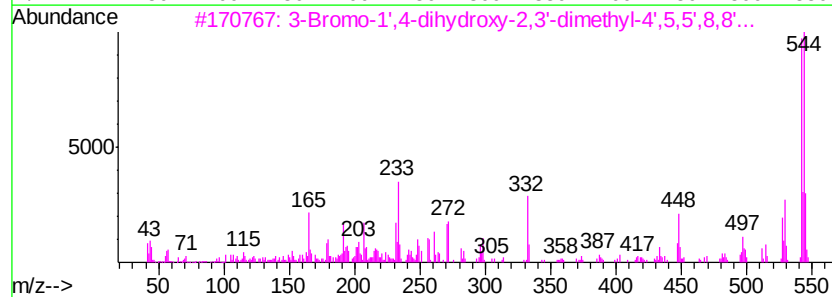
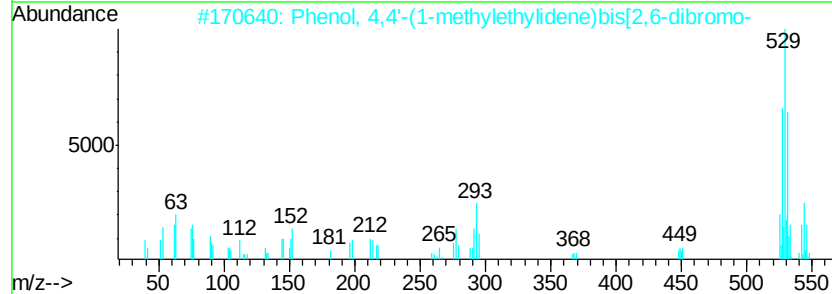
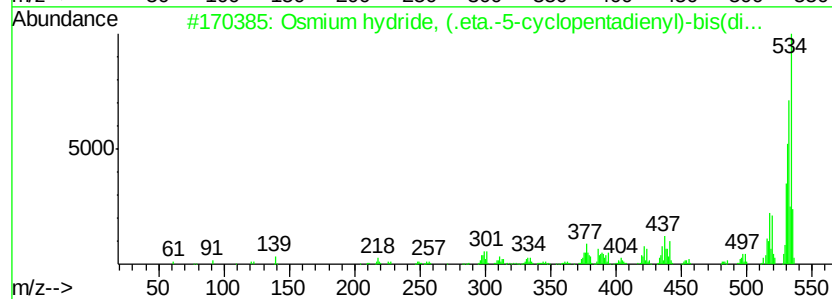
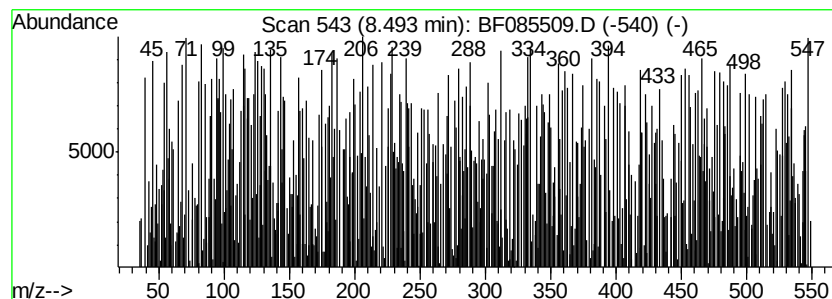
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown8.49 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.49	5.01 ng	294888	Napthalene-d8	8.16

Hit# of	3	Tentative ID	MW	MolForm	CAS#	Qual
1	Osmium hydride, (.eta.-5-cyclope...	534	C21H28OsP2	1000158-66-2	44	
2	Phenol, 4,4'-(1-methylethylidene...	540	C15H12Br4O2	000079-94-7	4	
3	3-Bromo-1',4-dihydroxy-2,3'-dime...	542	C27H27BrO7	101459-33-0	2	



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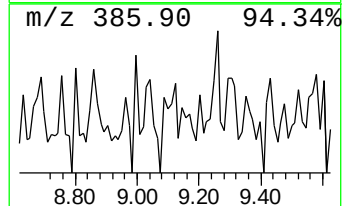
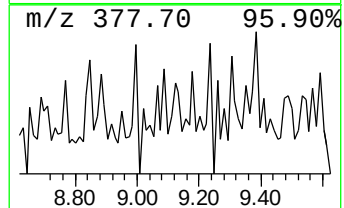
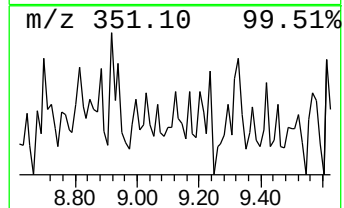
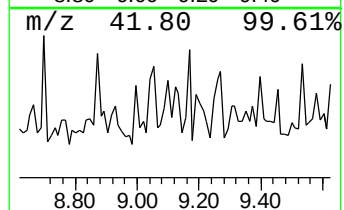
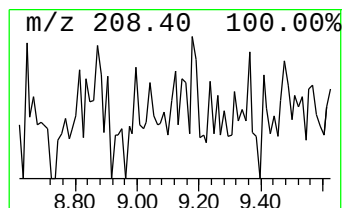
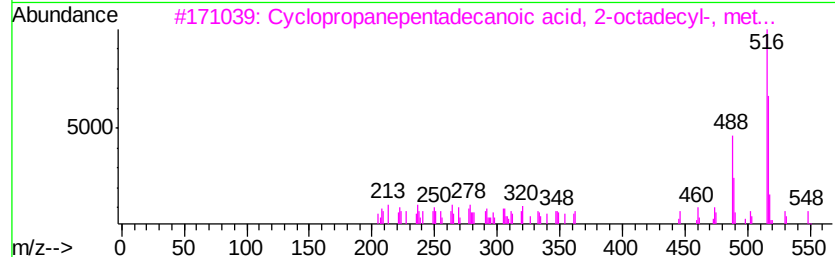
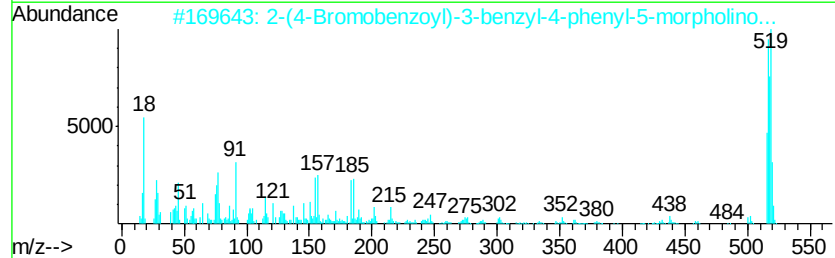
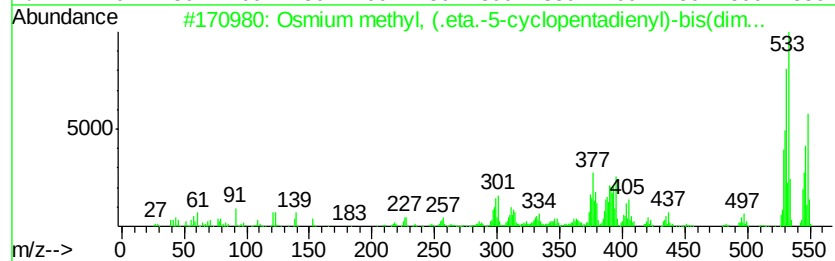
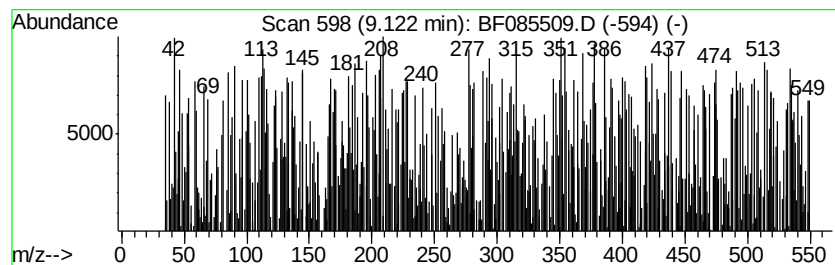
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Peak Number 9 unknown9.12 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
9.12	5.16 ng	300861	Acenaphthene-d10	9.91		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Osmium methyl, (.eta.-5-cyclopentenyl)-bis(dimethylamino)-	548	C22H30O2S	1000158-92-4	20	
2	2-(4-Bromobenzoyl)-3-benzyl-4-phenyl-5-morpholinol	517	C28H24BrN02S	1000286-90-3	10	
3	Cyclopropanepentadecanoic acid, 2-octadecyl-, methyl ester	549	C37H72O2	055517-72-1	9	
4	Phosphine, 4,6-dibenzofurandiylbis(2-methylphenyl)-	536	C36H26OP2	133850-81-4	7	
5	5-Isoxazolamine, N-methyl-N,3-diisopropyl-	532	C36H28N2OSi	135703-02-5	7	



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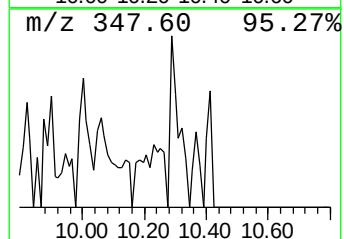
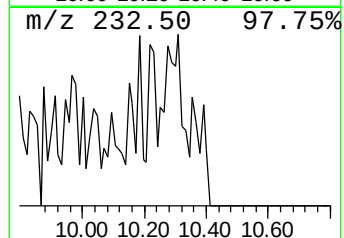
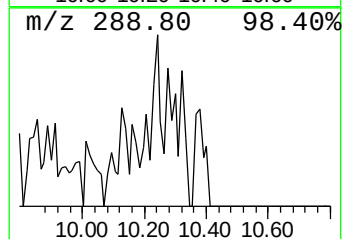
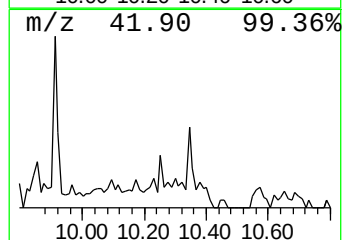
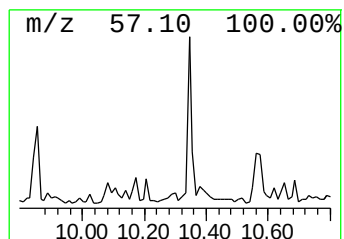
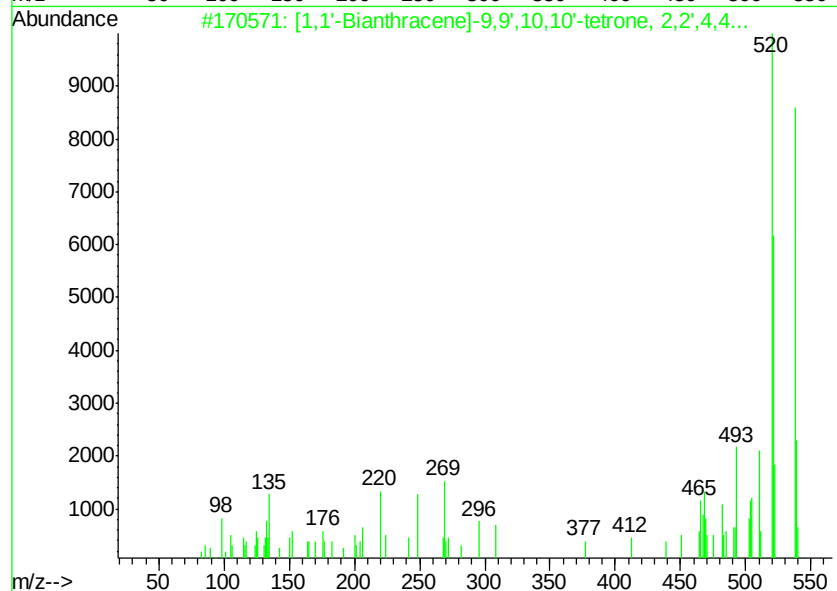
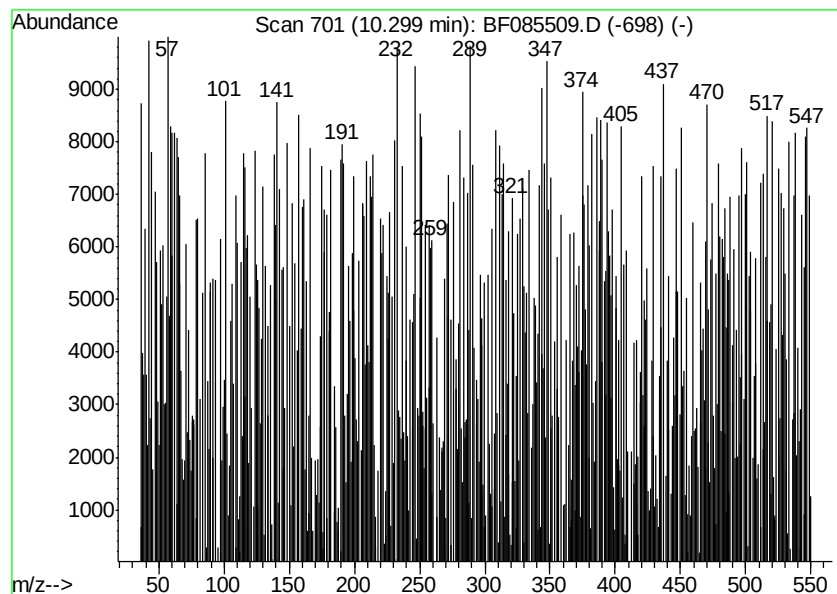
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown10.30 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.30	5.25 ng	306372	Acenaphthene-d10	9.91
Hit# of	1	Tentative ID	MW MolForm	CAS# Qual
1	[1,1'-Bianthracene]-9,9',10,10'-...	538 C30H18O10	000602-06-2	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085509.D
Acq On : 17 Mar 2016 23:41
Operator : UM/SJ
Sample : H1774-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

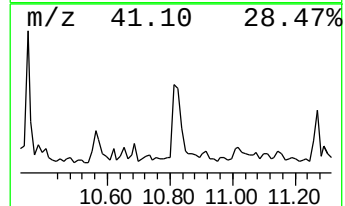
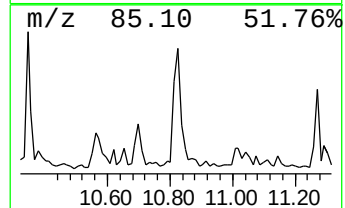
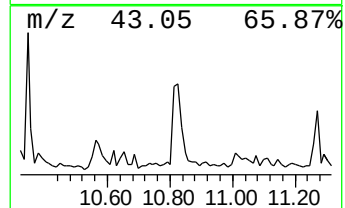
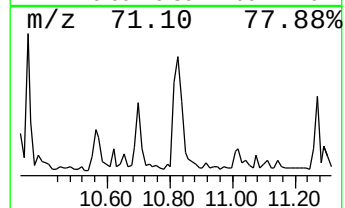
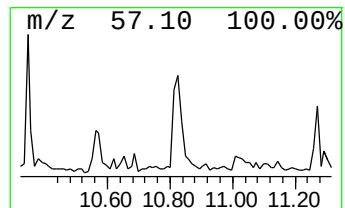
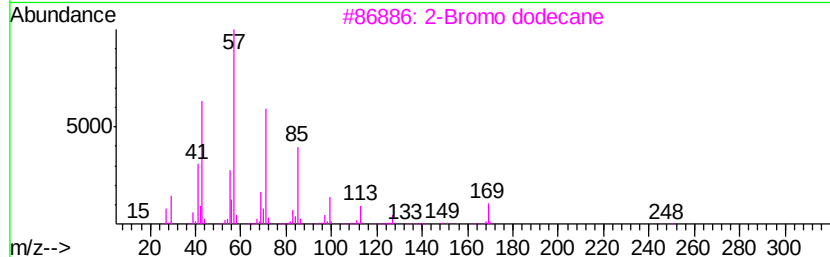
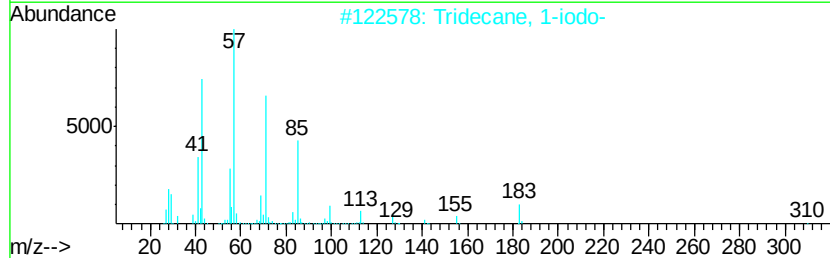
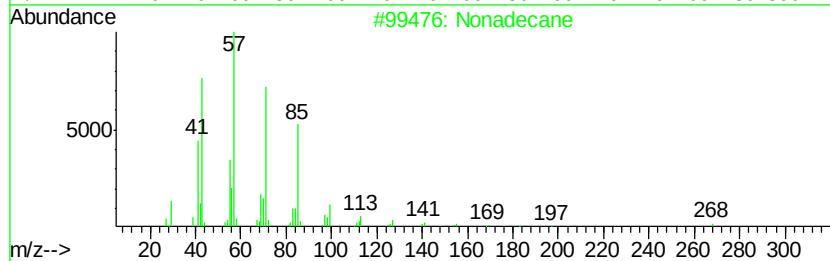
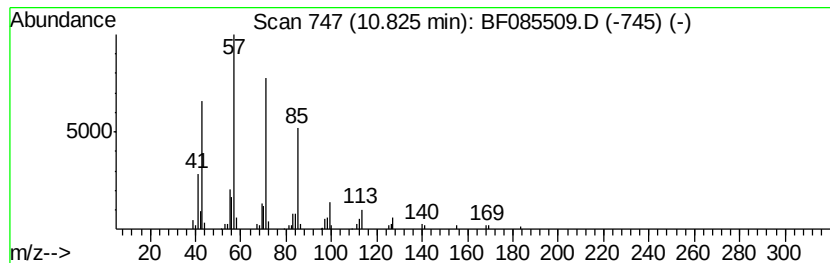
Instrument :
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ClientSampleId :
SB-23-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Nonadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.82	3.19 ng	181746	Phenanthrene-d10	11.40	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Octadecane	254	C18H38	000593-45-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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Acq On : 17 Mar 2016 23:41
Operator : UM/SJ
Sample : H1774-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

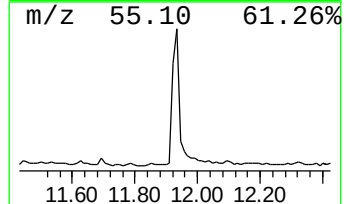
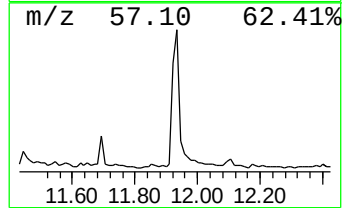
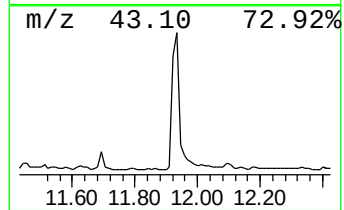
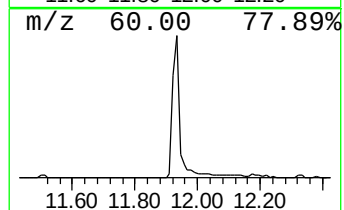
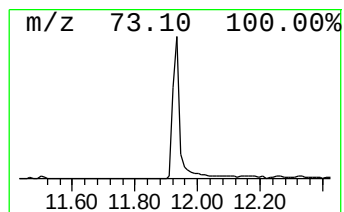
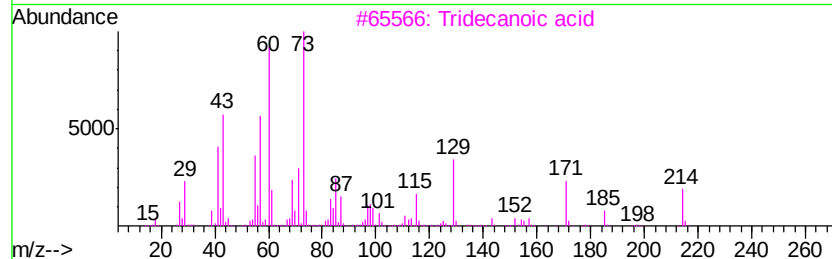
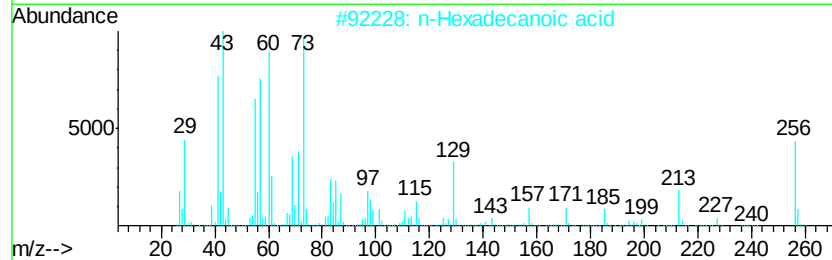
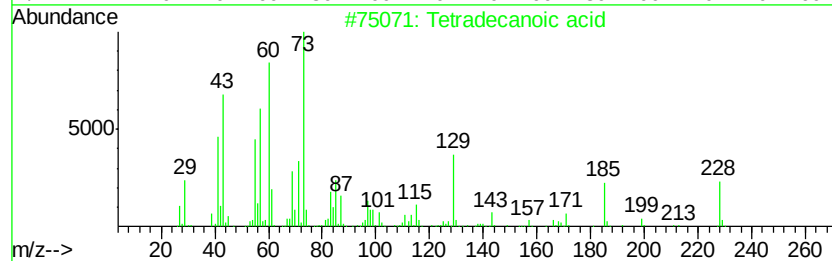
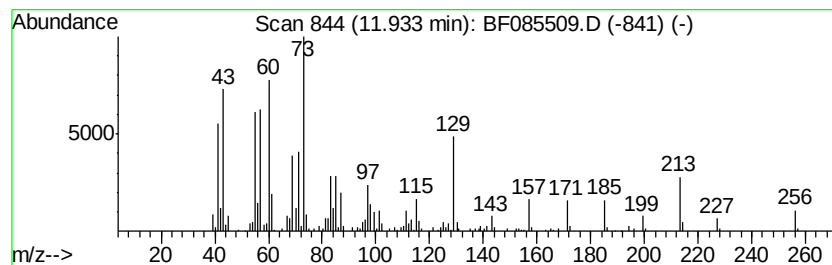
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetradecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.93	7.99 ng	455662	Phenanthrene-d10		11.40
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085509.D
Acq On : 17 Mar 2016 23:41
Operator : UM/SJ
Sample : H1774-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-23-COMP

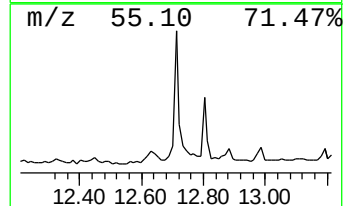
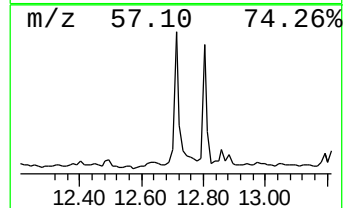
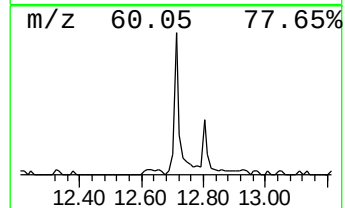
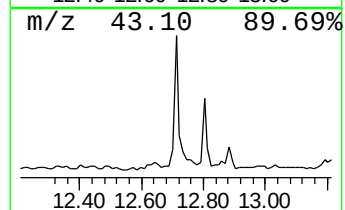
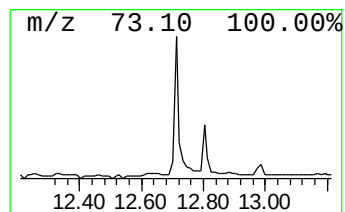
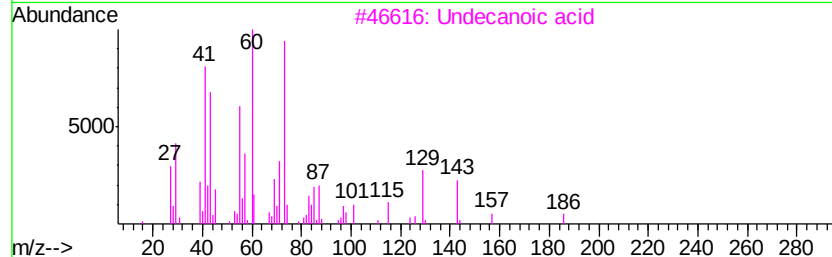
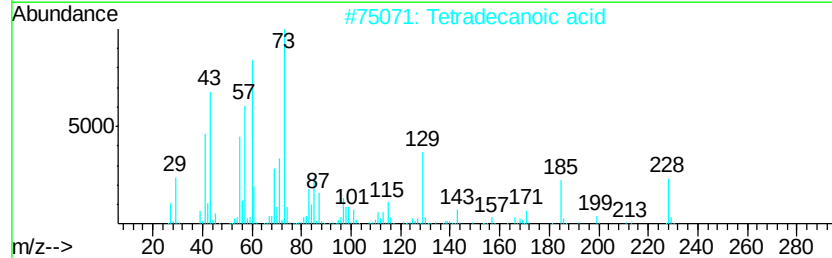
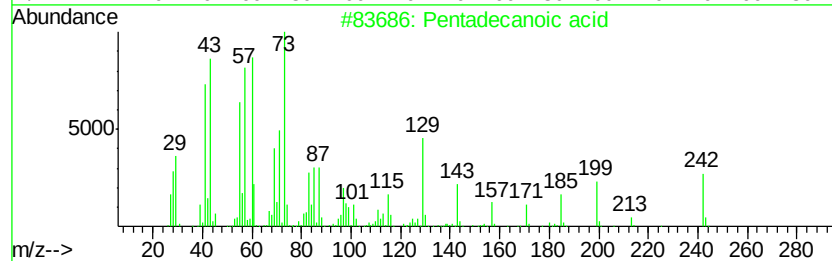
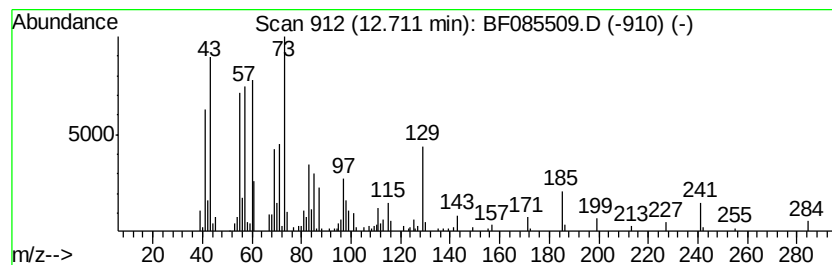
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Pentadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.58 ng	204404	Phenanthrene-d10	11.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3			Undecanoic acid	186	C11H22O2	000112-37-8	46
4			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38
5			Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
Data File : BF085509.D
Acq On : 17 Mar 2016 23:41
Operator : UM/SJ
Sample : H1774-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-23-COMP

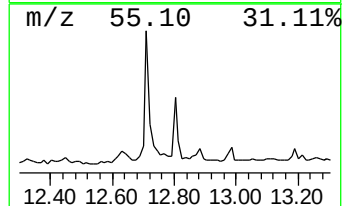
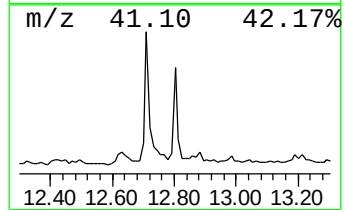
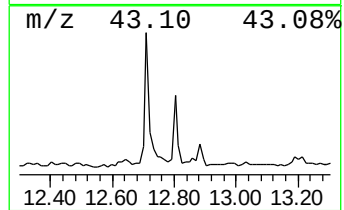
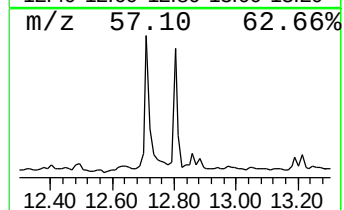
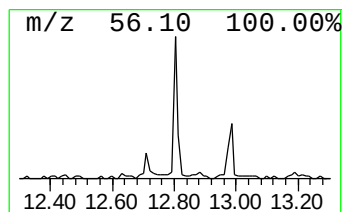
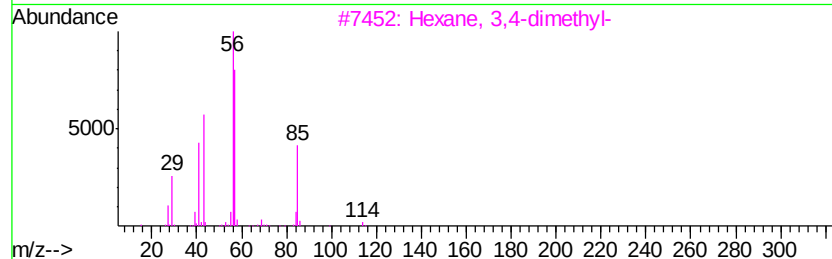
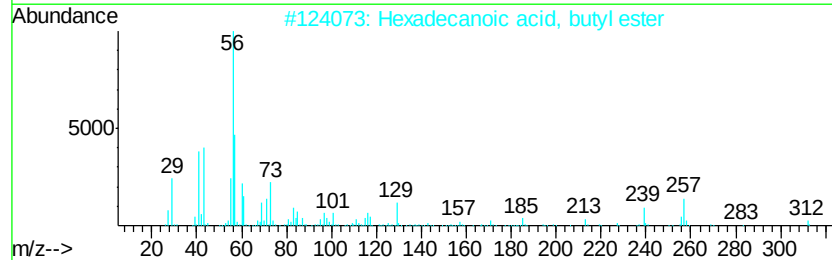
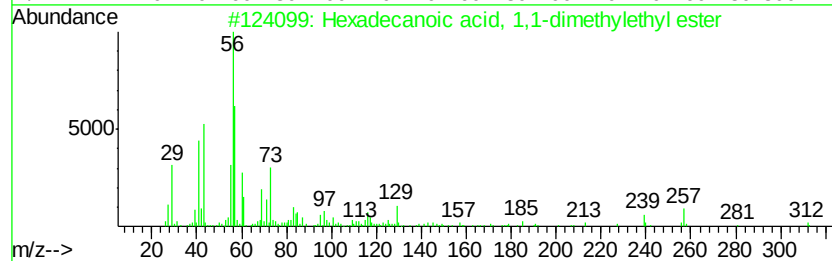
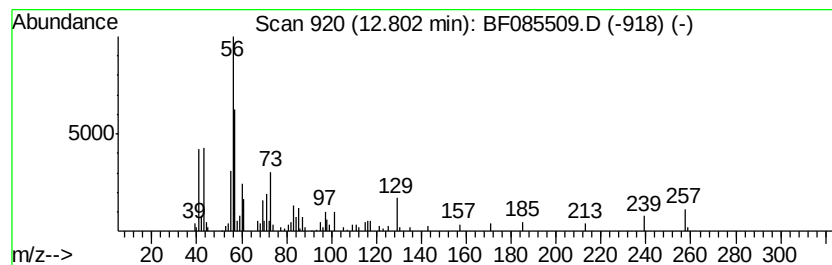
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Hexadecanoic acid, 1,1-dime... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.36 ng	110699	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
3		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
5		Cyclohexanol,2-amino-,trans-	115	C6H13NO	006982-39-4	30



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031716\
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Operator : UM/SJ
Sample : H1774-02
Misc :
ALS Vial : 31 Sample Multiplier: 1

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ClientSampleId :
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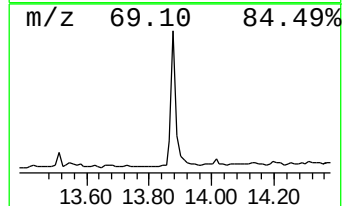
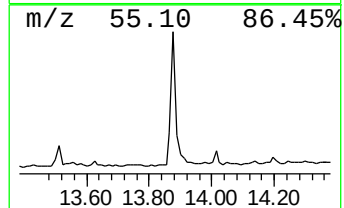
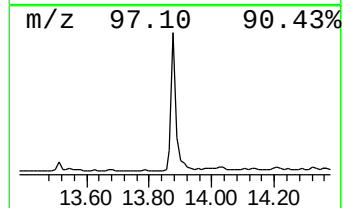
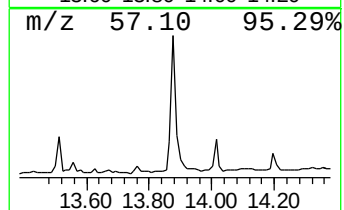
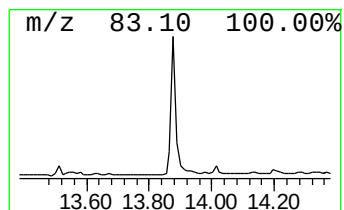
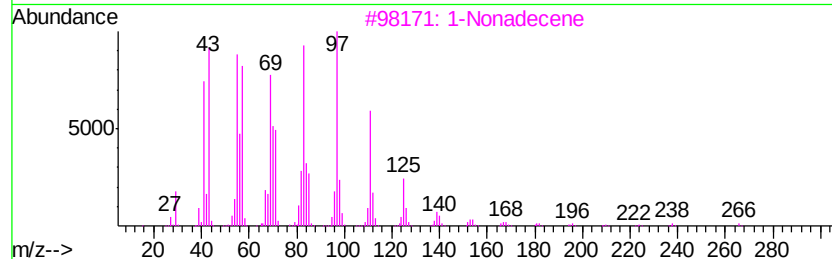
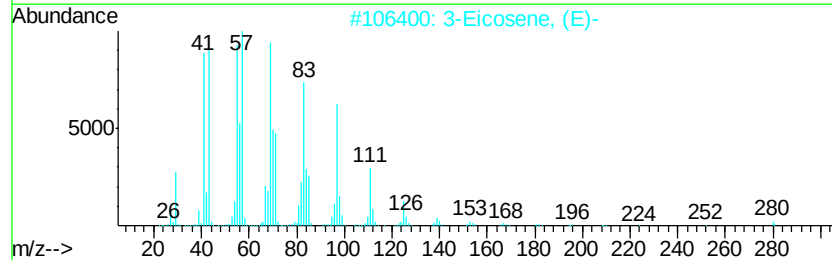
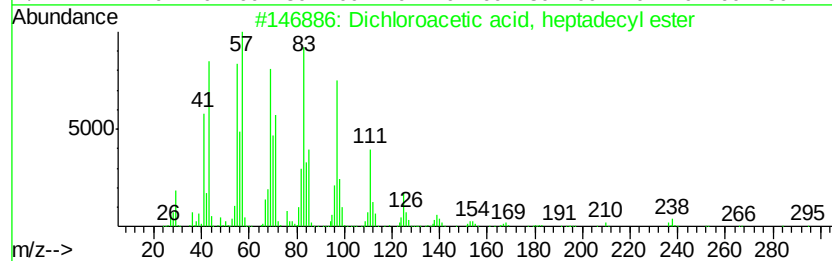
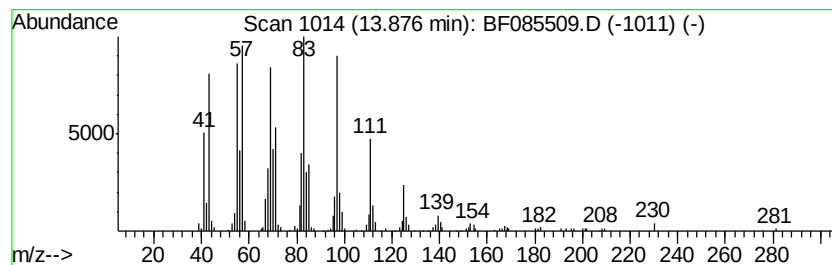
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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Peak Number 16 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	8.00 ng	375378	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
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unknown6.64	6.64	79.0	ng	3196520	1	6.87	808793	20.0
unknown8.49	8.49	5.0	ng	294888	2	8.16	1177230	20.0
unknown9.12	9.12	5.2	ng	300861	3	9.91	1166380	20.0
unknown10.30	10.30	5.3	ng	306372	3	9.91	1166380	20.0
Nonadecane	10.82	3.2	ng	181746	4	11.40	1140550	20.0
Tetradecanoic acid	11.93	8.0	ng	455662	4	11.40	1140550	20.0
Pentadecanoic acid	12.71	3.6	ng	204404	4	11.40	1140550	20.0
Hexadecanoic acid...	12.80	2.4	ng	110699	5	14.04	938970	20.0
Dichloroacetic ac...	13.88	8.0	ng	375378	5	14.04	938970	20.0