

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
 Data File : BF097050.D
 Acq On : 26 Jul 2017 1:02
 Operator : SJ/JU
 Sample : I4359-09
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CEMETERY-5-(0-2)

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-BF072517.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	2.675	131	134	142	rBV2	15109	40006	1.77%	0.207%
2	4.640	464	468	477	rBV	142730	194296	8.58%	1.004%
3	5.098	542	546	560	rBV	2008032	2076236	91.67%	10.724%
4	6.163	722	727	741	rBV	2103298	2264858	100.00%	11.699%
5	6.275	741	746	749	rBV	2162509	2056298	90.79%	10.621%
6	6.498	780	784	790	rBV	798951	670896	29.62%	3.465%
7	6.657	806	811	814	rBV	1578919	1462357	64.57%	7.554%
8	7.069	876	881	884	rBV	1399318	1271672	56.15%	6.569%
9	7.528	956	959	962	rBV	76394	60639	2.68%	0.313%
10	7.781	998	1002	1006	rBV	983311	849624	37.51%	4.389%
11	8.863	1181	1186	1189	rBV	2343269	2037014	89.94%	10.522%
12	9.192	1239	1242	1245	rBV	125269	97798	4.32%	0.505%
13	9.257	1248	1253	1257	rBV	264681	218855	9.66%	1.130%
14	9.463	1279	1288	1290	rBV4	14167	32284	1.43%	0.167%
15	9.527	1294	1299	1303	rVV	914257	789384	34.85%	4.077%
16	9.980	1374	1376	1380	rVB	38867	30862	1.36%	0.159%
17	10.204	1407	1414	1416	rBV2	17922	26900	1.19%	0.139%
18	10.310	1429	1432	1436	rBV	987642	940451	41.52%	4.858%
19	10.451	1453	1456	1463	rVB	58270	59093	2.61%	0.305%
20	10.898	1527	1532	1535	rBV3	32857	31192	1.38%	0.161%
21	10.998	1545	1549	1553	rBV	645159	599051	26.45%	3.094%
22	11.557	1640	1644	1651	rBV2	106705	106386	4.70%	0.550%
23	11.733	1671	1674	1681	rBV6	14224	24196	1.07%	0.125%
24	12.204	1751	1754	1757	rBV	40815	35208	1.55%	0.182%
25	12.333	1773	1776	1783	rBV3	30075	41896	1.85%	0.216%
26	12.427	1788	1792	1794	rBV	115125	103587	4.57%	0.535%
27	12.586	1815	1819	1822	rBV	1356807	1323740	58.45%	6.838%
28	12.821	1855	1859	1860	rBV3	22086	30962	1.37%	0.160%
29	13.010	1888	1891	1894	rBV2	35696	30566	1.35%	0.158%
30	13.045	1894	1897	1905	rVB4	54253	70249	3.10%	0.363%
31	13.133	1909	1912	1915	rBV2	46579	46134	2.04%	0.238%
32	13.492	1970	1973	1979	rVB2	114594	133131	5.88%	0.688%
33	13.621	1991	1995	1999	rBV	607911	573495	25.32%	2.962%
34	14.127	2078	2081	2088	rVB	80576	95590	4.22%	0.494%

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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	14.539	2149	2151	2154	rBV2	88543	69198	3.06%	0.357%
36	14.709	2176	2180	2187	rBV2	114899	184238	8.13%	0.952%
37	14.974	2221	2225	2229	rBV	334280	363158	16.03%	1.876%
38	15.386	2291	2295	2300	rBV	228183	318435	14.06%	1.645%

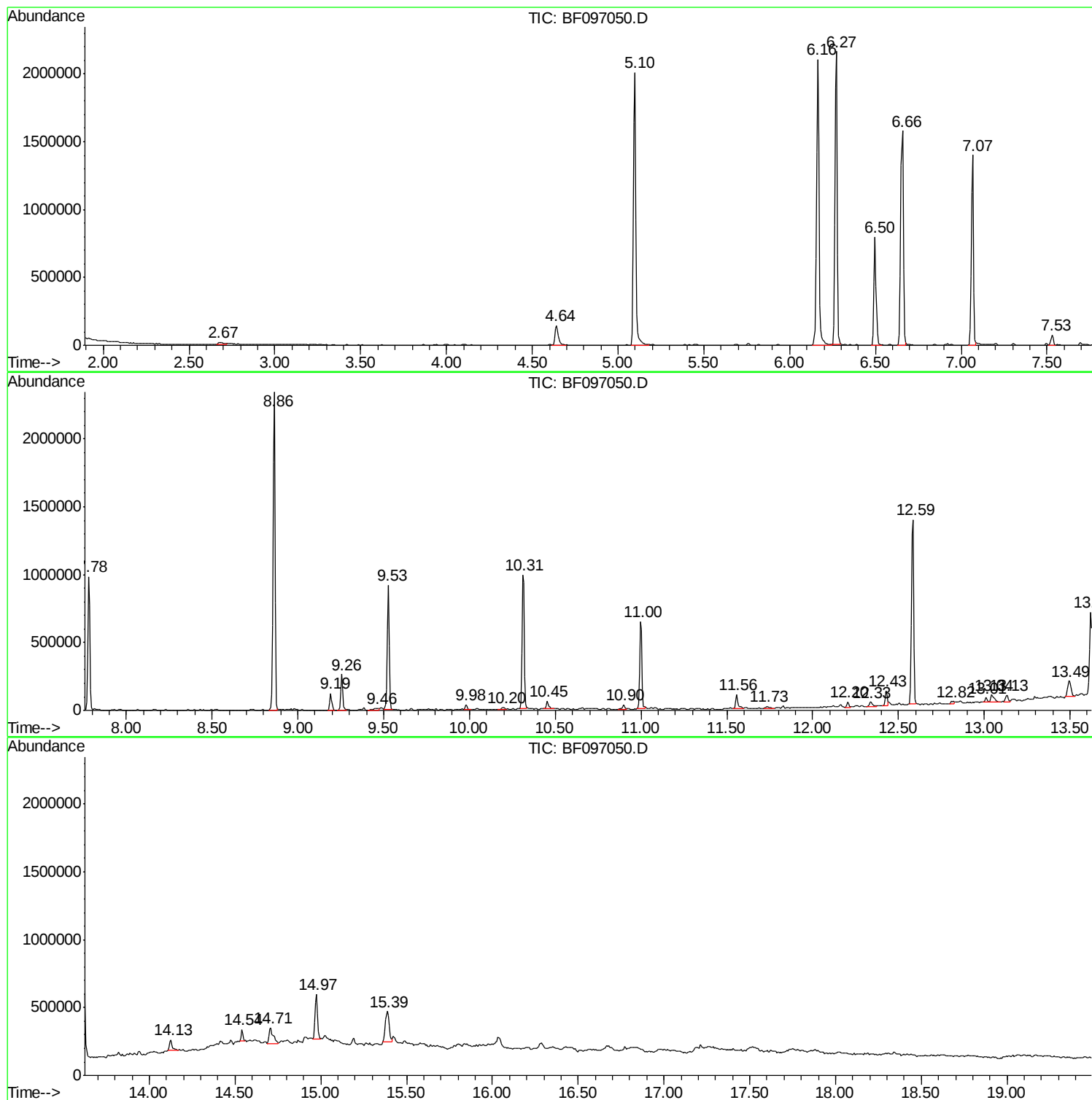
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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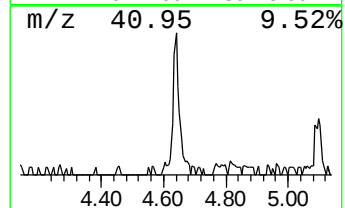
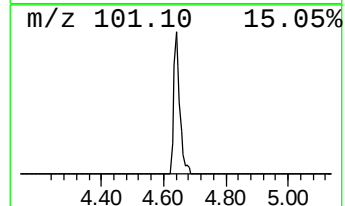
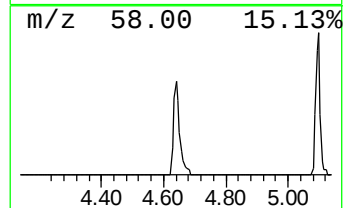
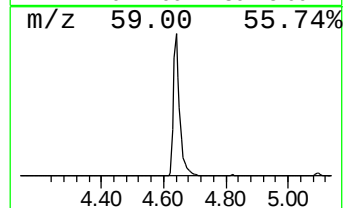
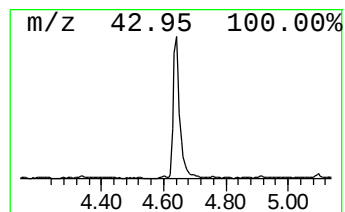
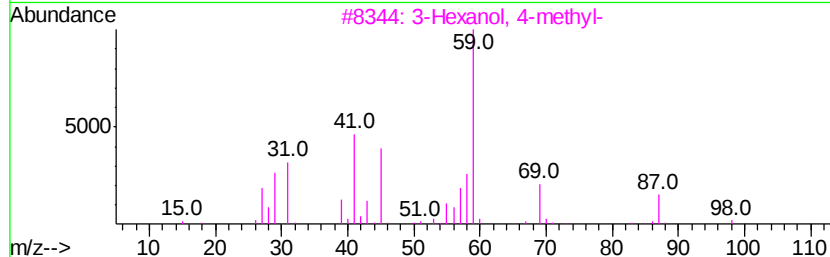
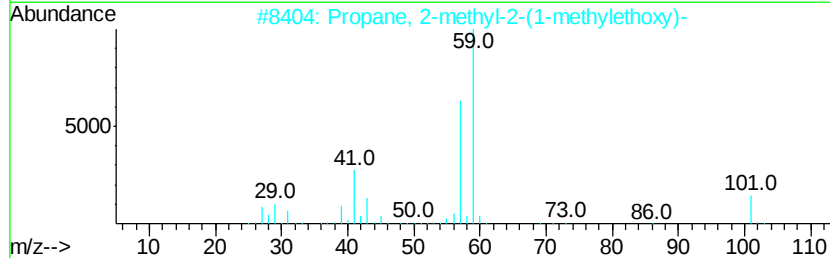
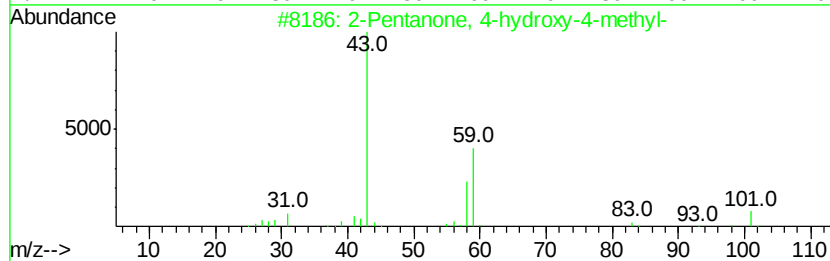
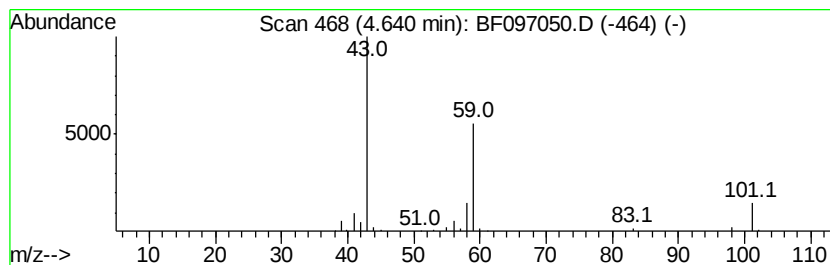
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.64	5.79 ng	194296	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	25



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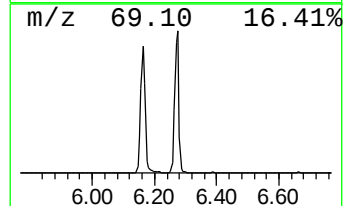
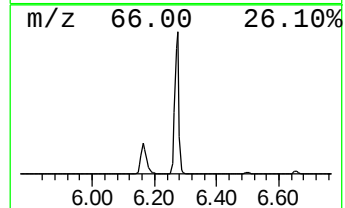
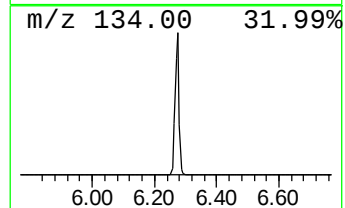
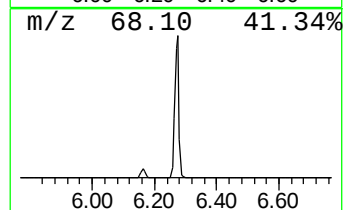
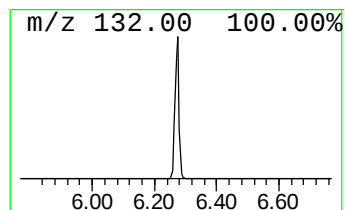
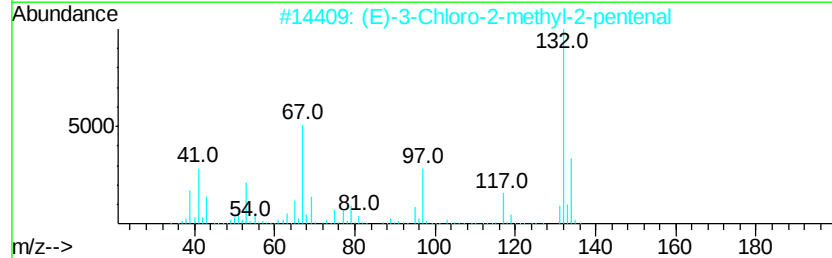
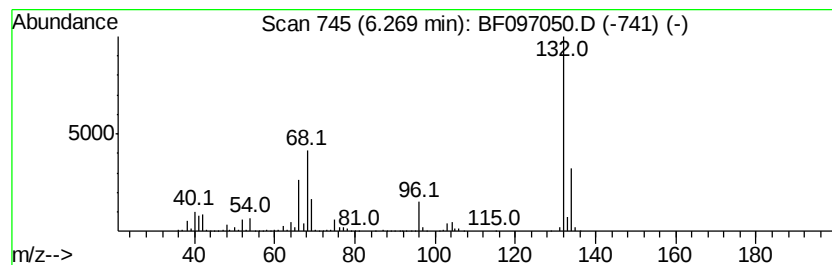
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	61.30 ng	2056300	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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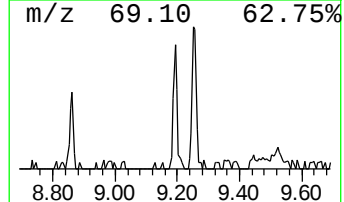
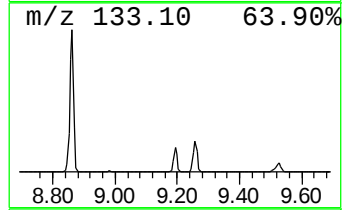
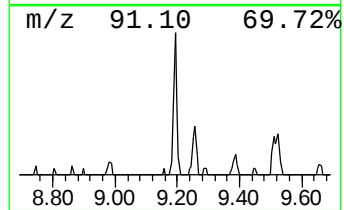
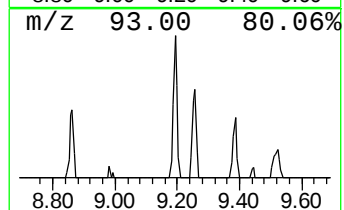
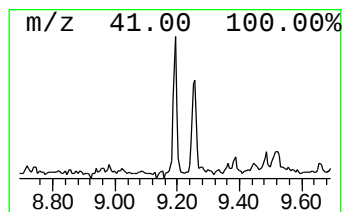
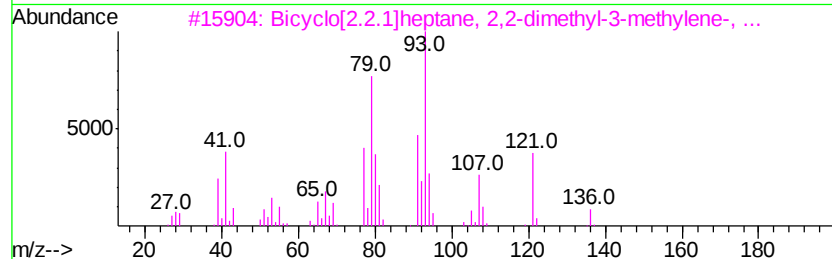
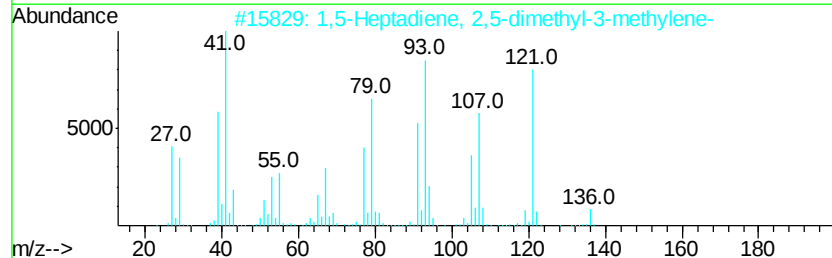
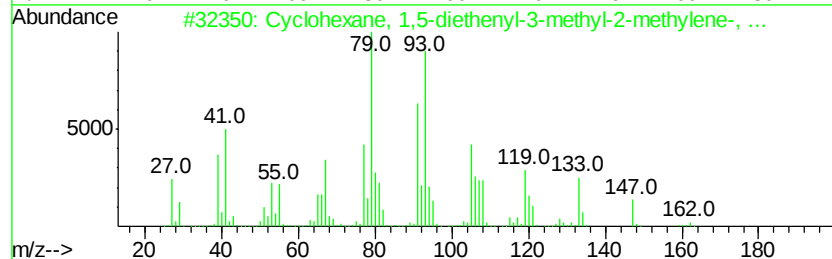
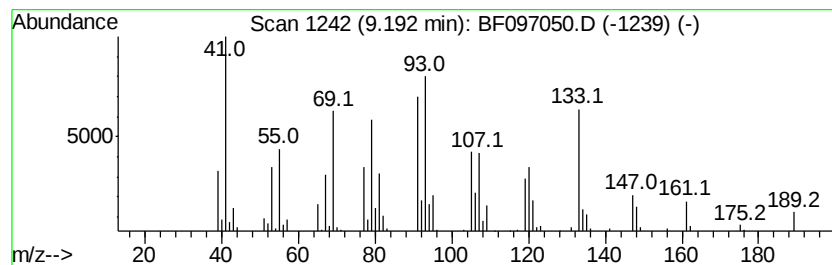
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 4 Cyclohexane, 1,5-diethenyl-... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.19	2.48 ng	97798	Acenaphthene-d10	9.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,5-diethenyl-3-met...	162	C12H18	074742-35-1	76
2		1,5-Heptadiene, 2,5-dimethyl-3-m...	136	C10H16	074663-83-5	38
3		Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-03-6	38
4		Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	35
5		Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	35



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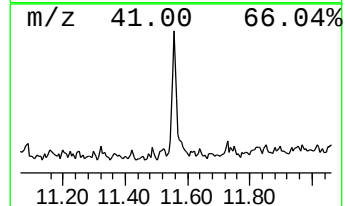
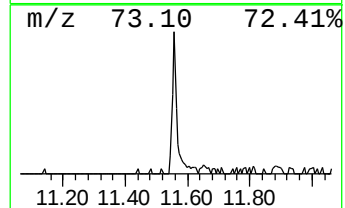
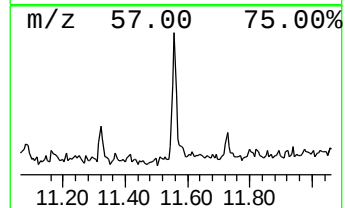
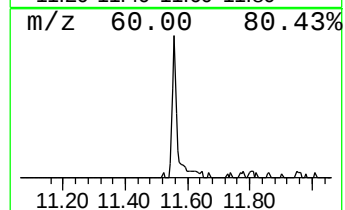
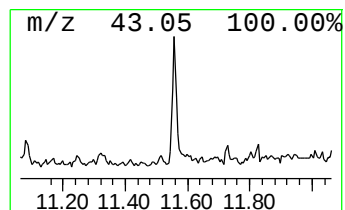
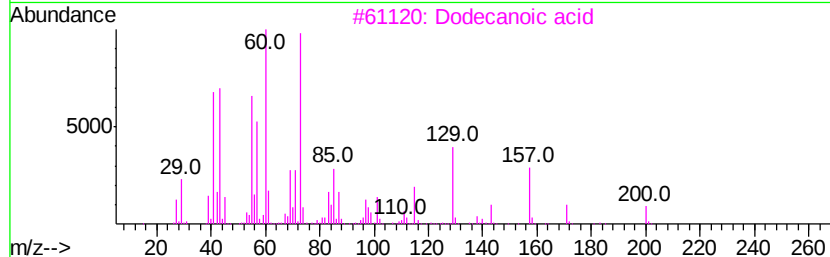
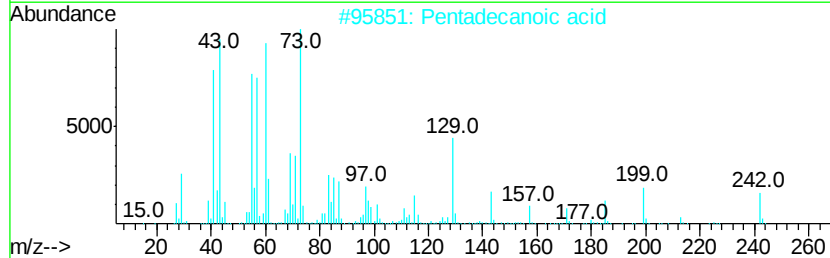
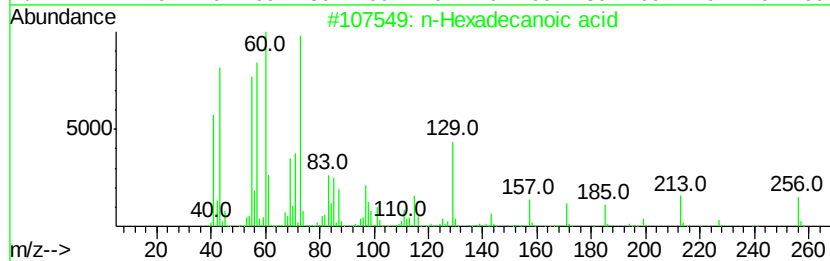
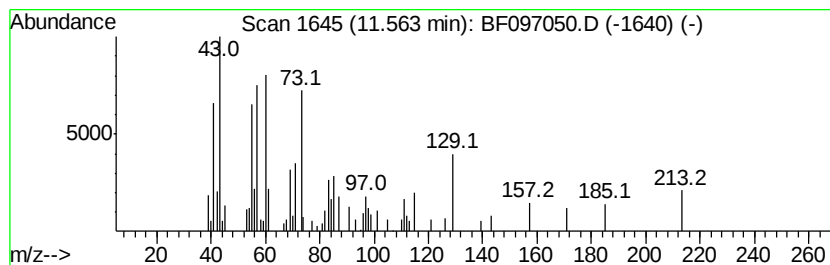
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	3.55 ng	106386	Phenanthrene-d10	11.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3		Dodecanoic acid	200	C12H24O2	000143-07-7	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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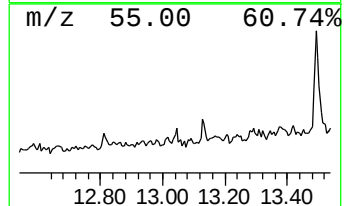
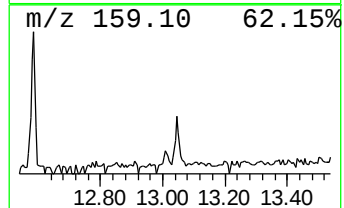
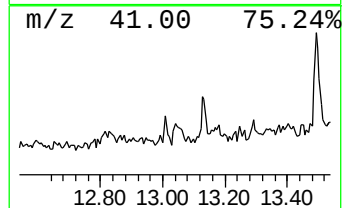
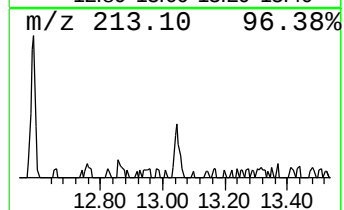
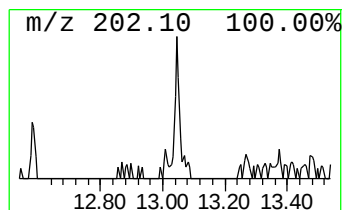
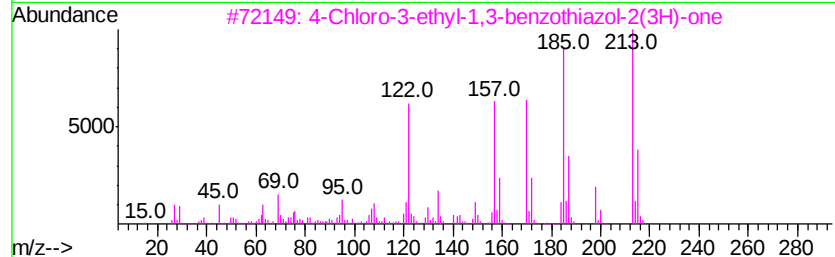
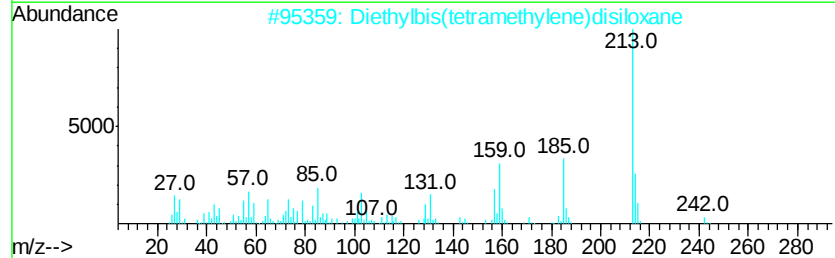
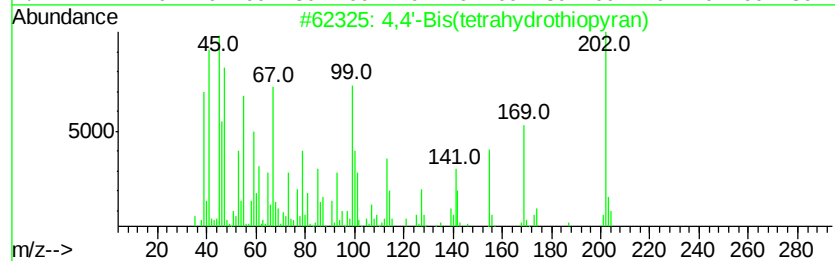
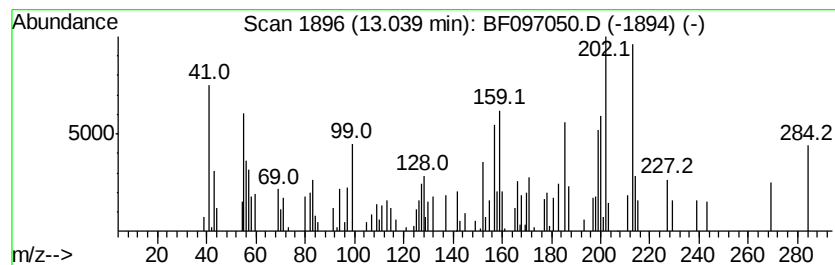
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Peak Number 7 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.04	2.45 ng	70249	Chrysene-d12	13.62		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'	-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	90
2	Diethylbis(tetramethylene)disilo...		242	C12H26OSi2	018035-51-3	27
3	4-Chloro-3-ethyl-1,3-benzothiazo...		213	C9H8ClNOS	1000331-84-8	25
4	9-Borabicyclo[3.3.1]nonane, 9-br...		200	C8H14BBr	022086-45-9	20
5	1,3,4-Trimethyl-6-cyclohexylbenzene		202	C15H22	032406-17-0	20



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072517\
Data File : BF097050.D
Acq On : 26 Jul 2017 1:02
Operator : SJ/JU
Sample : I4359-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

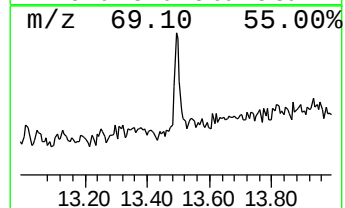
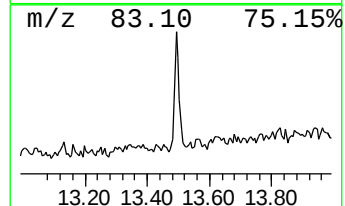
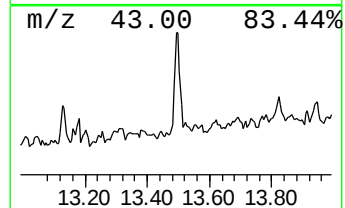
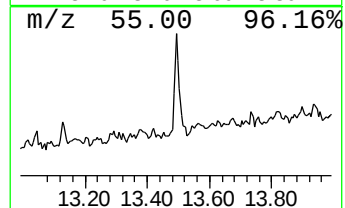
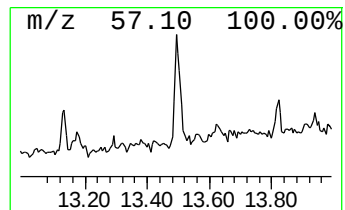
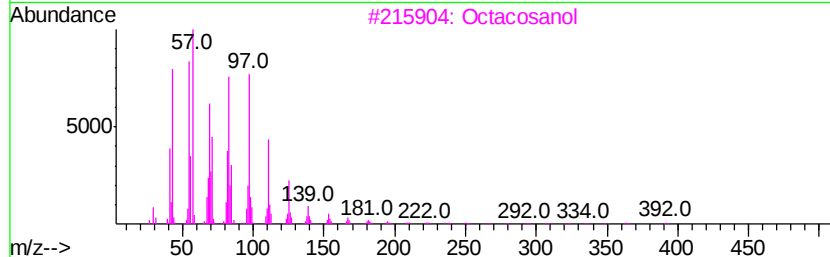
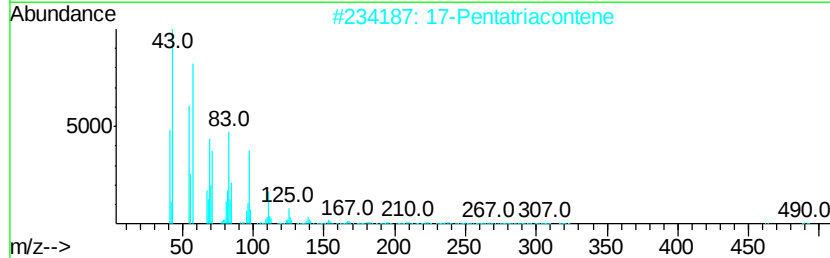
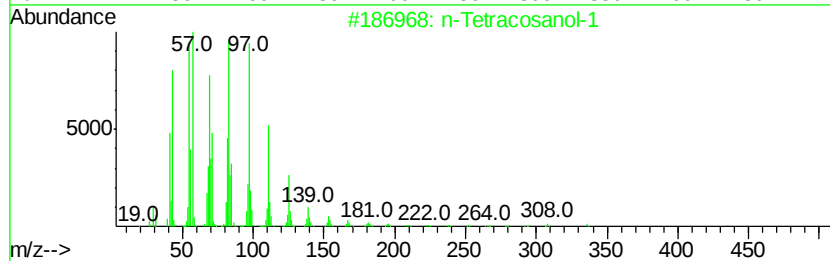
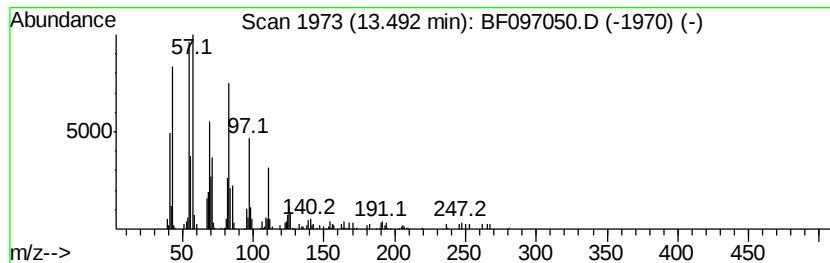
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.49	4.64 ng	133131	Chrysene-d12	13.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	17-Pentatriacontene	491	C35H70	006971-40-0	87
3	Octacosanol	410	C28H58O	000557-61-9	87
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	86
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097050.D
Acq On : 26 Jul 2017 1:02
Operator : SJ/JU
Sample : I4359-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CEMETERY-5-(0-2)

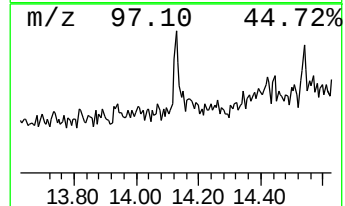
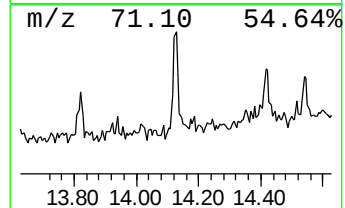
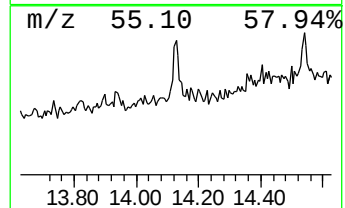
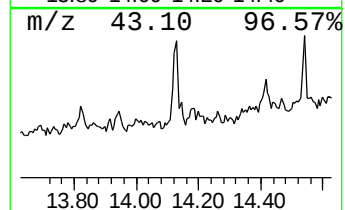
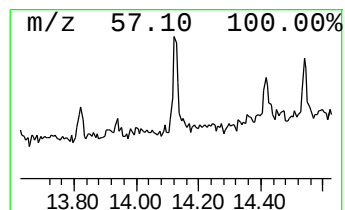
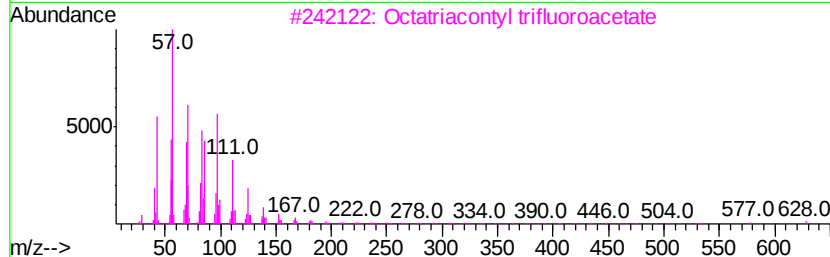
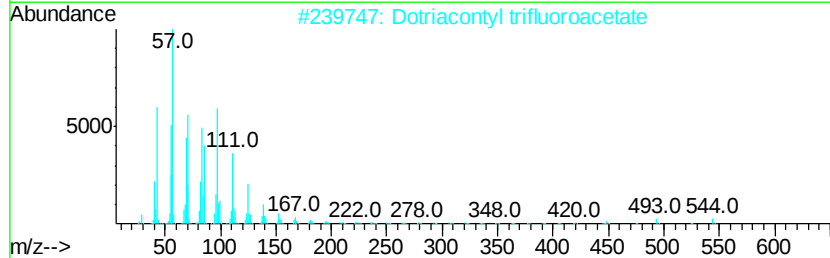
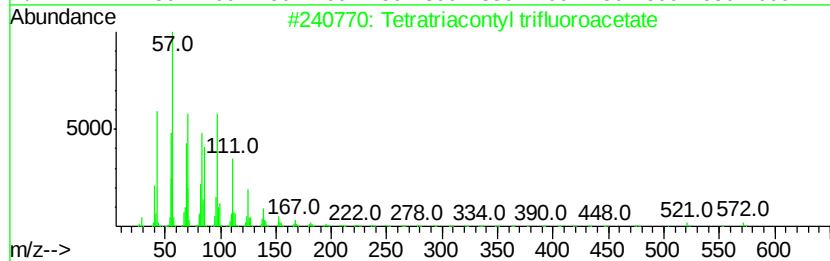
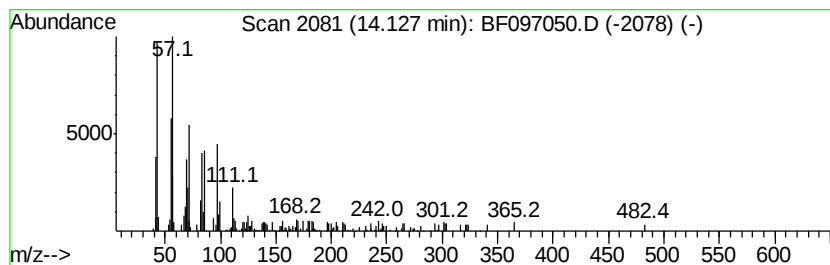
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Tetratriacontyl trifluoroac... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.13	3.33 ng	95590	Chrysene-d12	13.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	83
2		Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	83
3		Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	83
4		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	83
5		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	83



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072517\
Data File : BF097050.D
Acq On : 26 Jul 2017 1:02
Operator : SJ/JU
Sample : I4359-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

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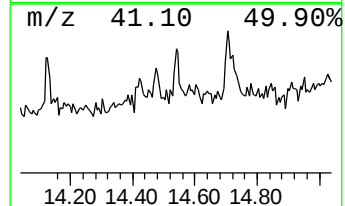
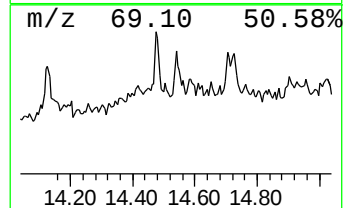
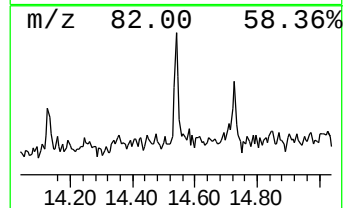
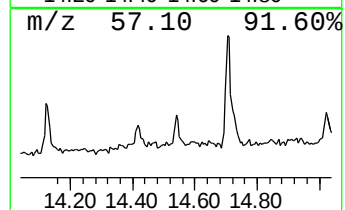
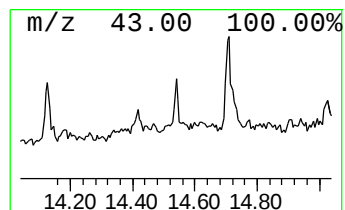
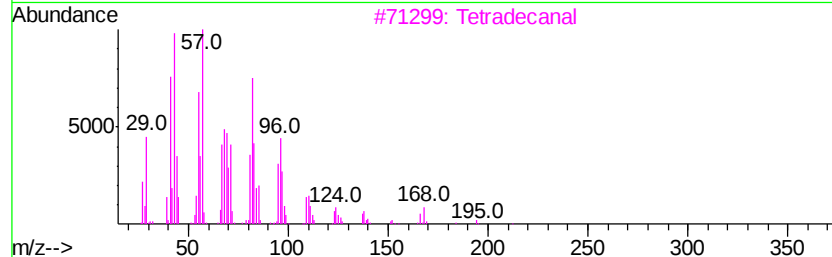
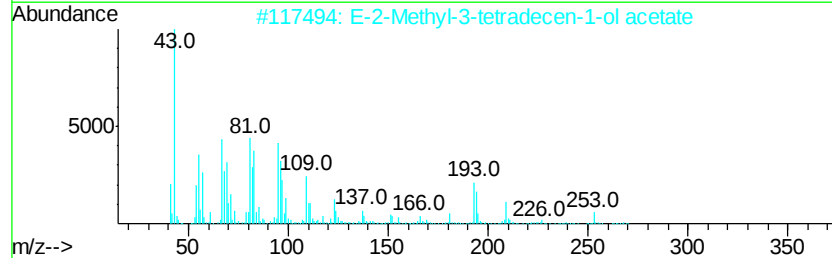
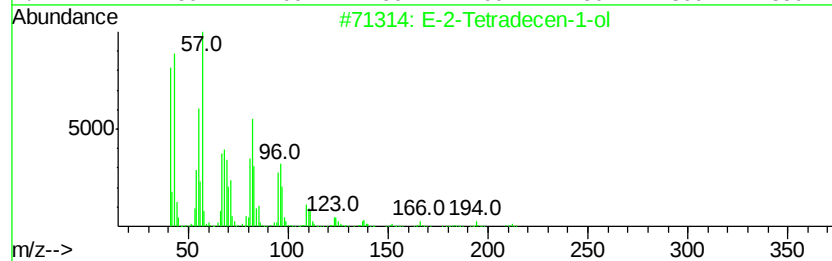
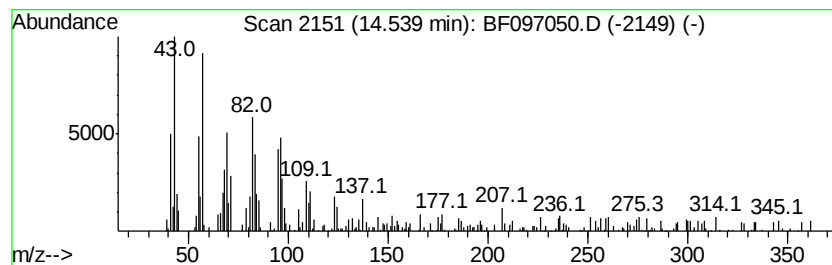
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 E-2-Tetradecen-1-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.81 ng	69198	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-2-Tetradecen-1-ol	212	C14H28O	1000130-83-7	90
2		E-2-Methyl-3-tetradecen-1-ol ace...	268	C17H32O2	1000130-81-2	89
3		Tetradecanal	212	C14H28O	000124-25-4	87
4		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	86
5		Octadecanal	268	C18H36O	000638-66-4	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072517\
Data File : BF097050.D
Acq On : 26 Jul 2017 1:02
Operator : SJ/JU
Sample : I4359-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CEMETERY-5-(0-2)

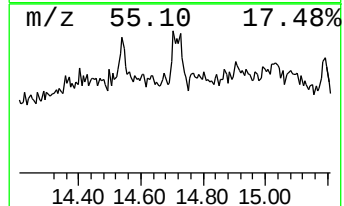
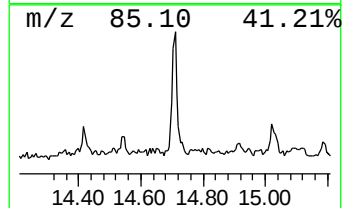
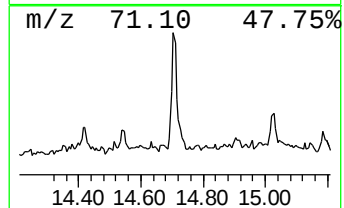
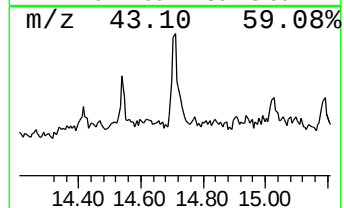
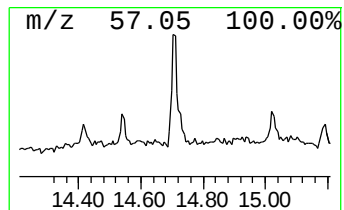
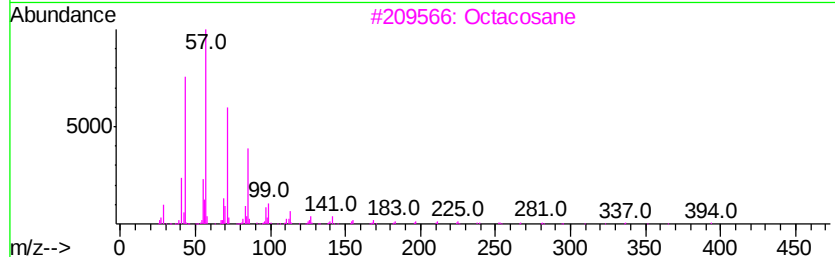
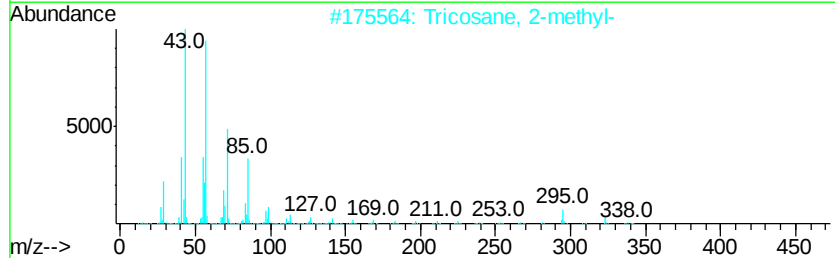
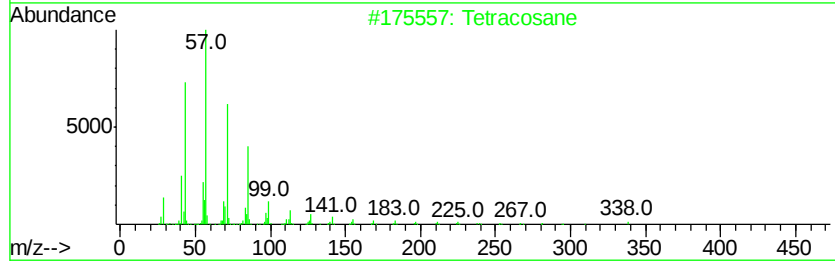
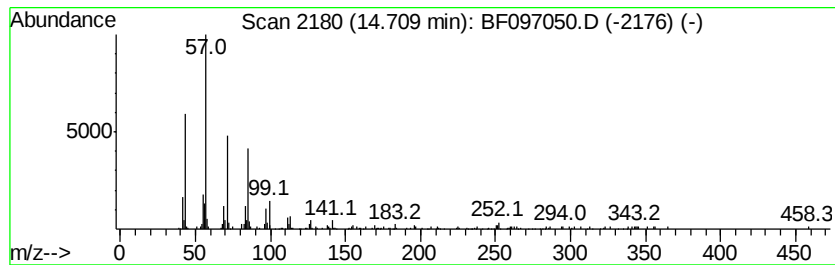
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	10.15 ng	184238	Perylene-d12	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	91
2		Tricosane, 2-methyl-	338	C24H50	001928-30-9	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Tetratetracontane	619	C44H90	007098-22-8	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
Data File : BF097050.D
Acq On : 26 Jul 2017 1:02
Operator : SJ/JU
Sample : I4359-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

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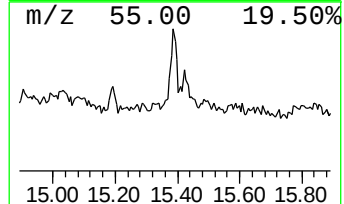
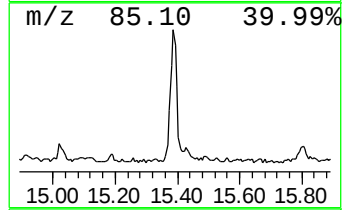
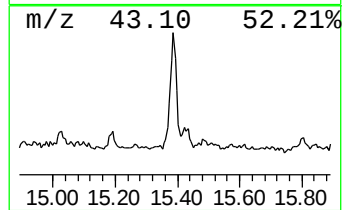
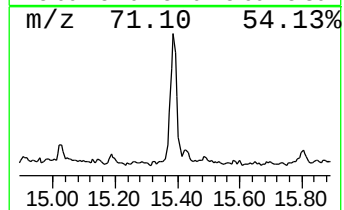
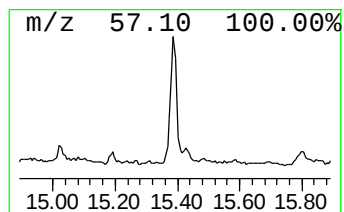
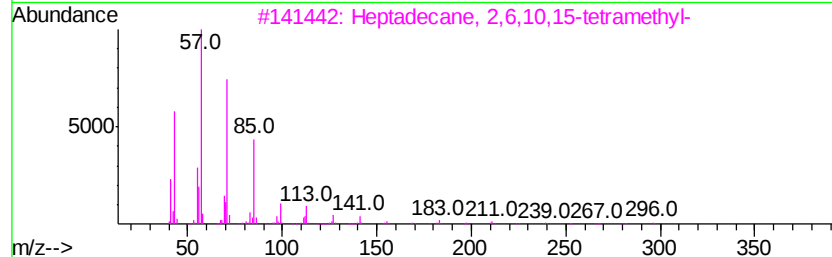
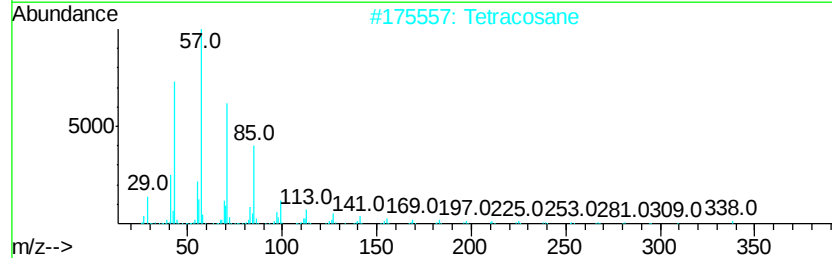
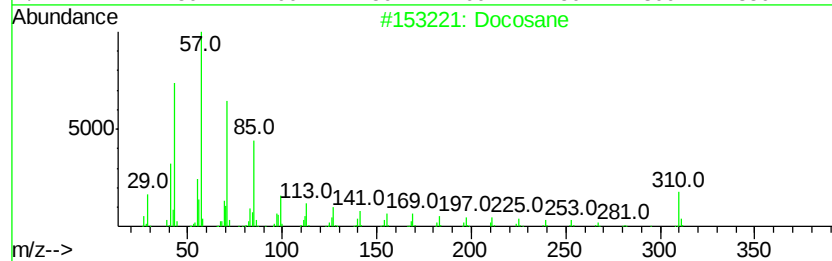
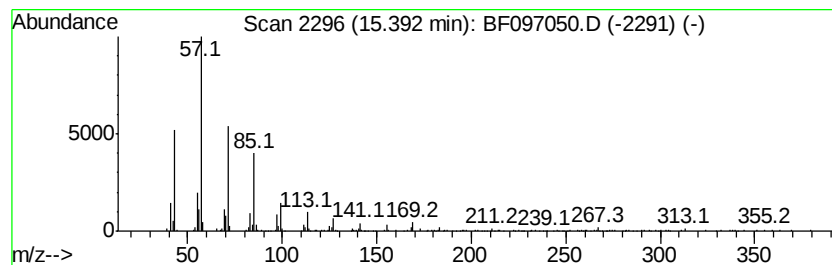
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Docosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	17.54 ng	318435	Perylene-d12	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	93
2			Tetracosane	338	C24H50	000646-31-1	90
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
4			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87
5			Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072517\
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Acq On : 26 Jul 2017 1:02
Operator : SJ/JU
Sample : I4359-09
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CEMETERY-5-(0-2)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown6.27	6.27	61.3	ng	2056300	1	6.50	670896	20.0
Cyclohexane, 1,5-...	9.19	2.5	ng	97798	3	9.53	789384	20.0
n-Hexadecanoic acid	11.56	3.5	ng	106386	4	11.00	599051	20.0
4,4'-Bis(tetrahyd...	13.04	2.5	ng	70249	5	13.62	573495	20.0
n-Tetracosanol-1	13.49	4.6	ng	133131	5	13.62	573495	20.0
Tetratriacontyl t...	14.13	3.3	ng	95590	5	13.62	573495	20.0
E-2-Tetradecen-1-ol	14.54	3.8	ng	69198	6	14.97	363158	20.0
Tetracosane	14.71	10.2	ng	184238	6	14.97	363158	20.0
Docosane	15.39	17.5	ng	318435	6	14.97	363158	20.0