

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
 Data File : BF098889.D
 Acq On : 28 Sep 2017 3:37
 Operator : SJ/JU
 Sample : I5396-02
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-B

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-BF092317.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	2.228	19	24	31	rVB	102002	131529	3.53%	0.397%
2	2.575	74	83	88	rVB2	17817	41740	1.12%	0.126%
3	4.034	325	331	336	rBV	108708	141236	3.79%	0.427%
4	5.151	516	521	533	rBV	533352	727991	19.52%	2.199%
5	5.539	581	587	590	rBV	3398874	3610382	96.82%	10.905%
6	6.545	752	758	766	rBV	3141372	3728921	100.00%	11.263%
7	6.686	777	782	785	rBV	3695238	3619357	97.06%	10.933%
8	6.916	817	821	824	rVB	1199957	949021	25.45%	2.867%
9	7.075	843	848	851	rBV	2813433	2543481	68.21%	7.683%
10	7.475	911	916	920	rBV	2056653	2195699	58.88%	6.632%
11	8.198	1035	1039	1042	rBV	1526609	1293891	34.70%	3.908%
12	9.275	1216	1222	1225	rBV	3461537	3517317	94.33%	10.624%
13	9.663	1284	1288	1291	rBV	699368	598434	16.05%	1.808%
14	9.951	1333	1337	1341	rBV	1444681	1319438	35.38%	3.985%
15	10.374	1402	1409	1411	rBV	56954	55537	1.49%	0.168%
16	10.745	1464	1472	1475	rBV	1900354	1993465	53.46%	6.021%
17	10.845	1486	1489	1498	rVB	72757	98641	2.65%	0.298%
18	11.439	1586	1590	1593	rBV	1418396	1193550	32.01%	3.605%
19	11.951	1674	1677	1684	rBV3	49155	50729	1.36%	0.153%
20	12.833	1824	1827	1830	rBV	180219	142587	3.82%	0.431%
21	12.910	1838	1840	1844	rVB	51729	41177	1.10%	0.124%
22	13.027	1855	1860	1863	rBV	2568393	2537275	68.04%	7.664%
23	13.539	1944	1947	1950	rBV	132222	101314	2.72%	0.306%
24	13.586	1950	1955	1957	rBV2	28837	43741	1.17%	0.132%
25	13.904	2006	2009	2018	rBV	175182	192761	5.17%	0.582%
26	14.080	2035	2039	2042	rVV	1098815	947427	25.41%	2.862%
27	14.533	2113	2116	2120	rBV2	54198	59845	1.60%	0.181%
28	14.845	2167	2169	2174	rVB	43116	39267	1.05%	0.119%
29	15.192	2225	2228	2231	rBV	64329	68352	1.83%	0.206%
30	15.574	2287	2293	2302	rVB	591971	827553	22.19%	2.500%
31	16.033	2367	2371	2376	rVB2	68807	104659	2.81%	0.316%
32	16.551	2455	2459	2464	rVB3	61864	115687	3.10%	0.349%
33	17.168	2559	2564	2569	rVB3	38541	74294	1.99%	0.224%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

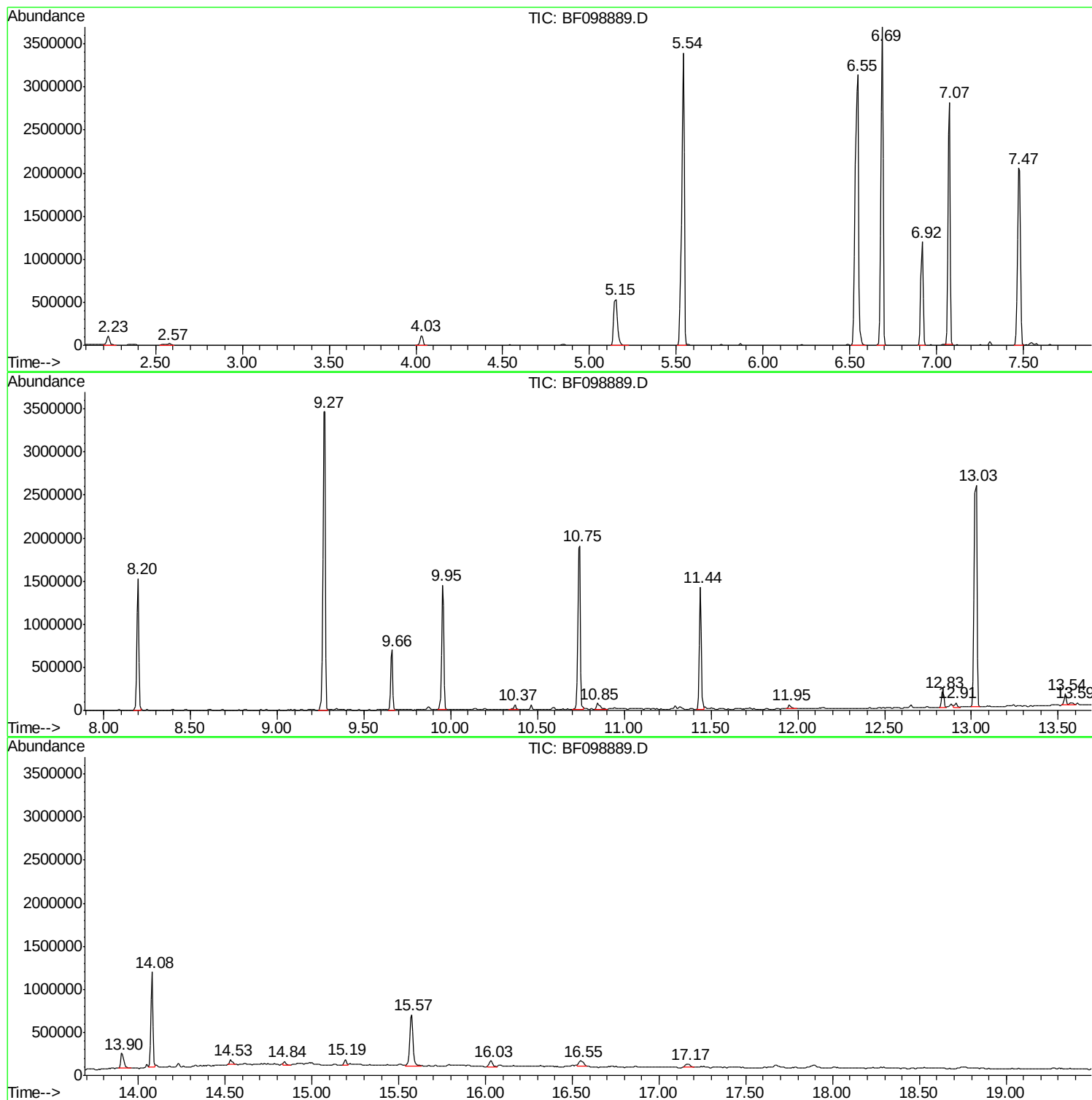
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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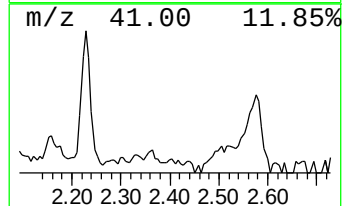
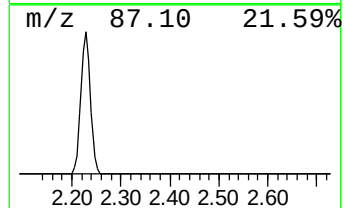
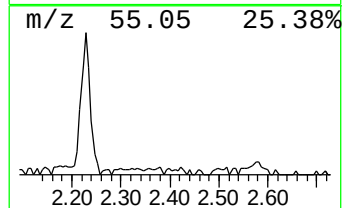
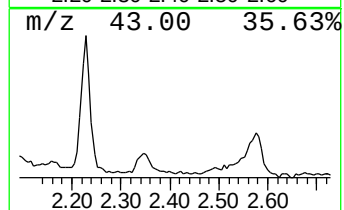
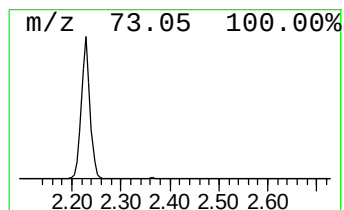
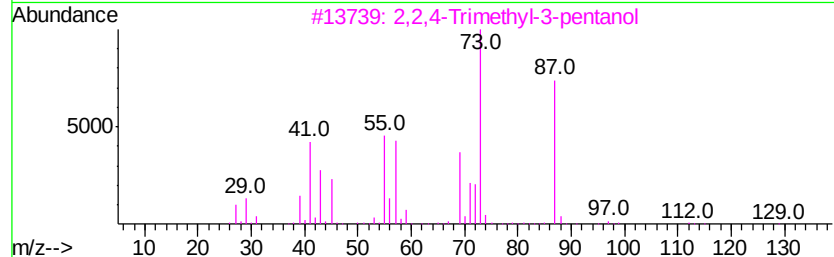
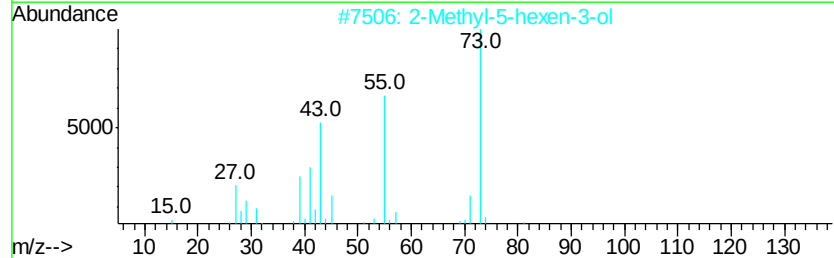
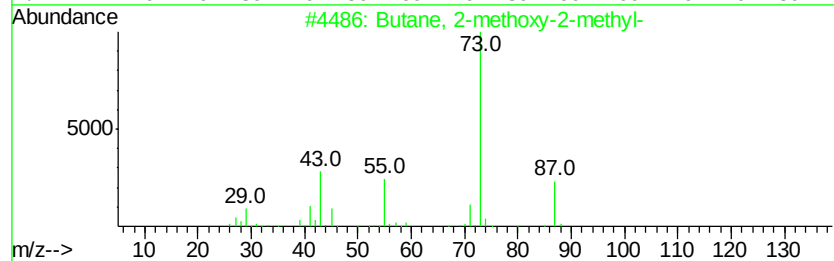
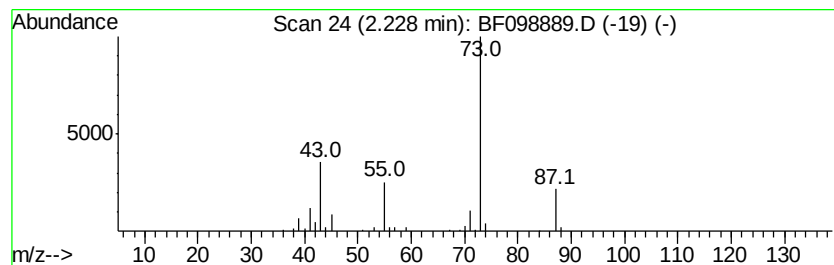
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	2.77 ng	131529	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25



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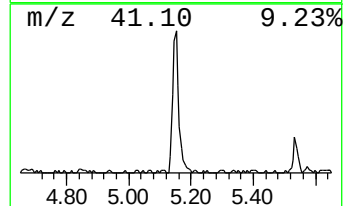
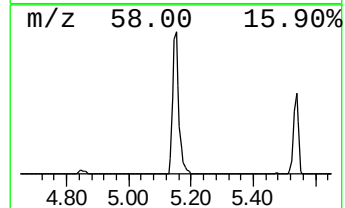
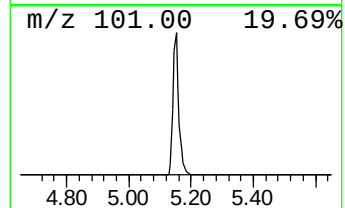
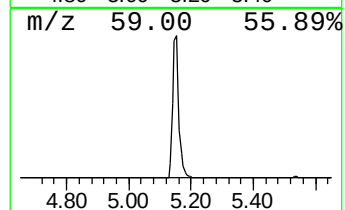
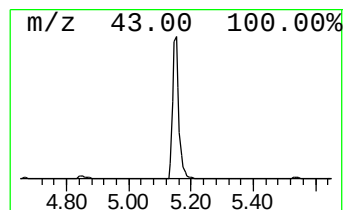
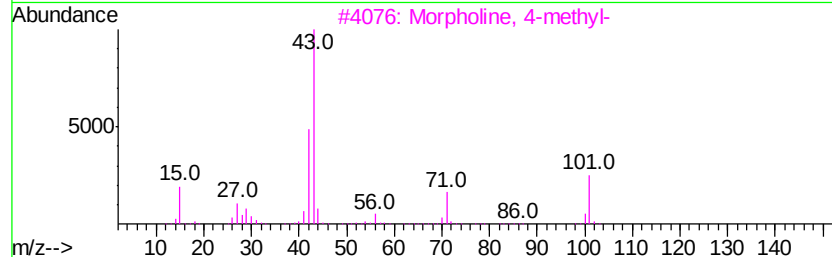
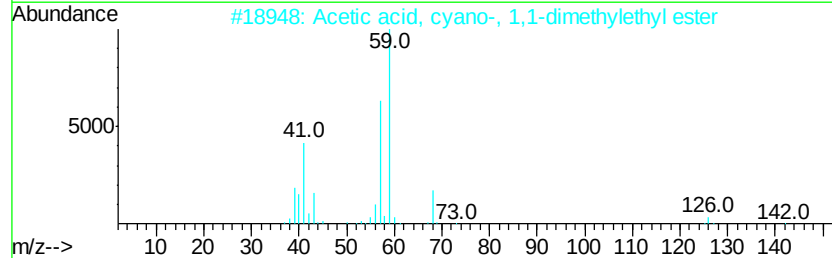
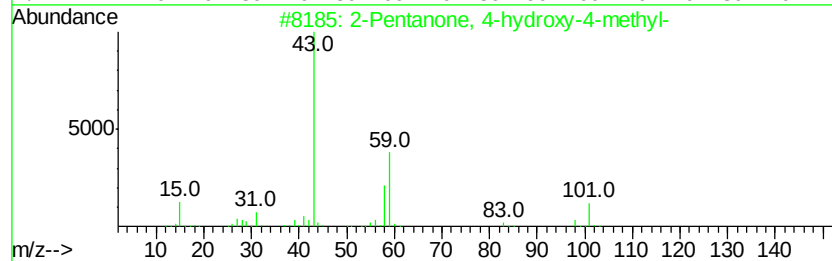
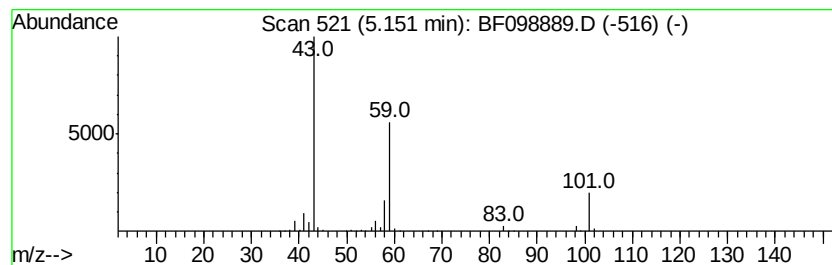
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	15.34 ng	727991	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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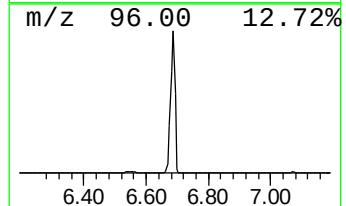
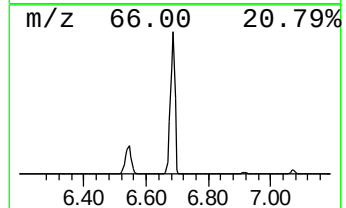
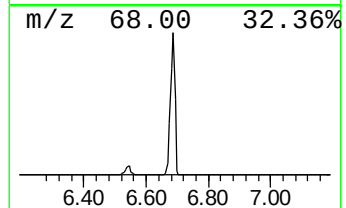
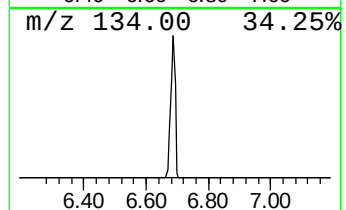
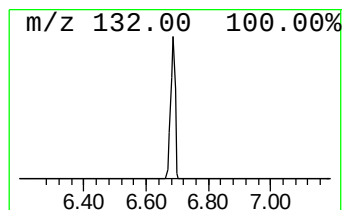
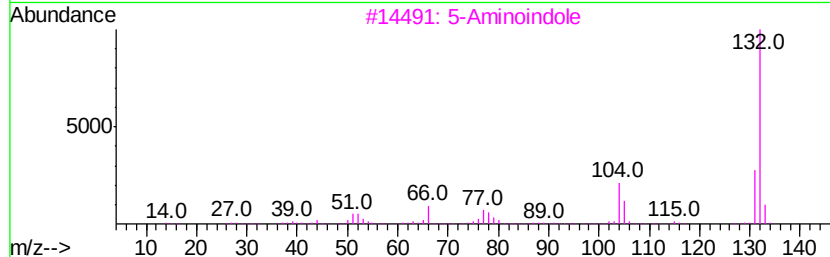
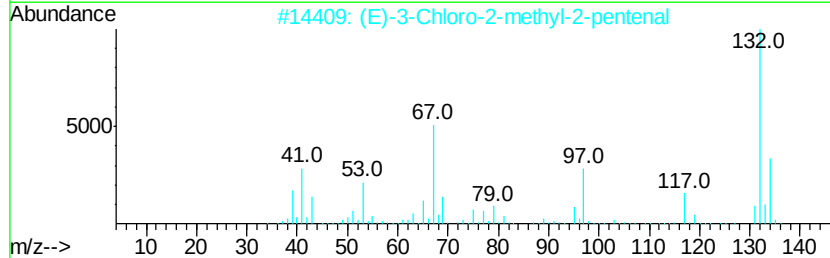
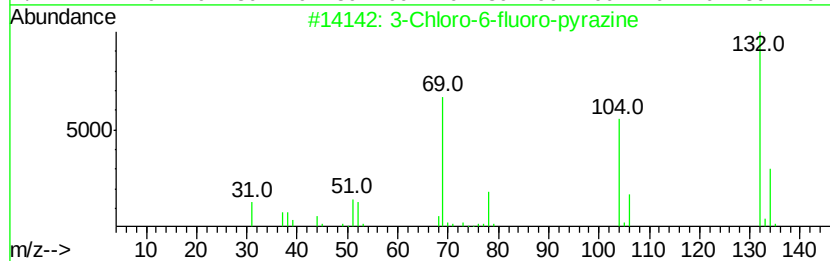
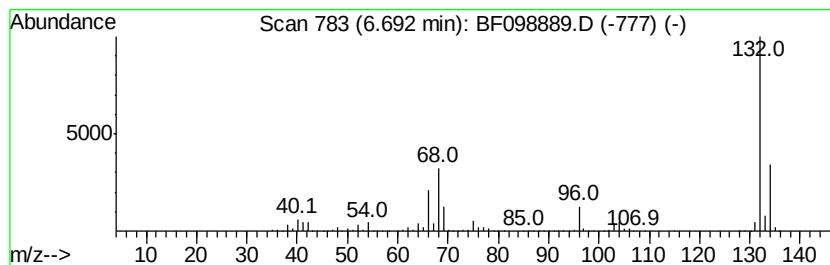
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	76.28 ng	3619360	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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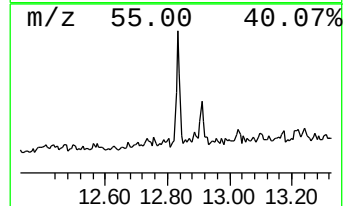
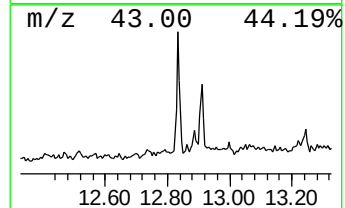
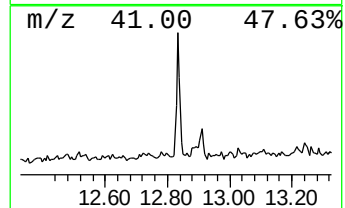
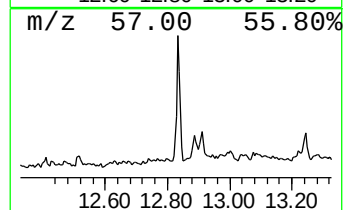
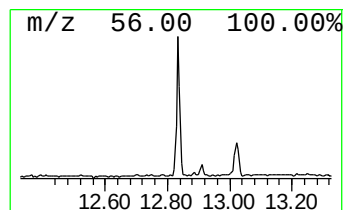
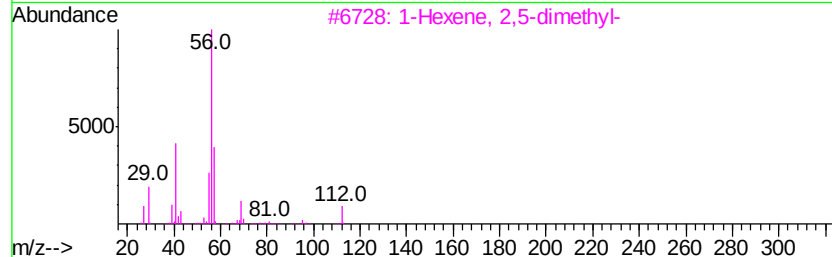
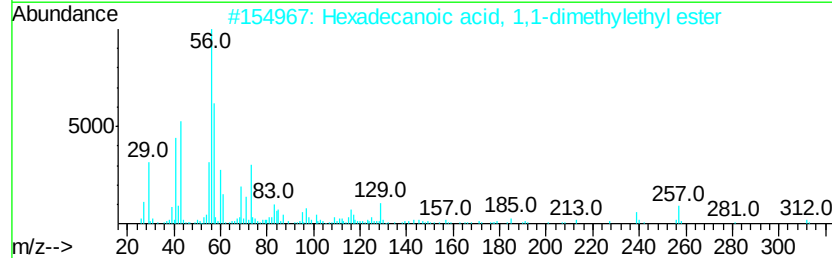
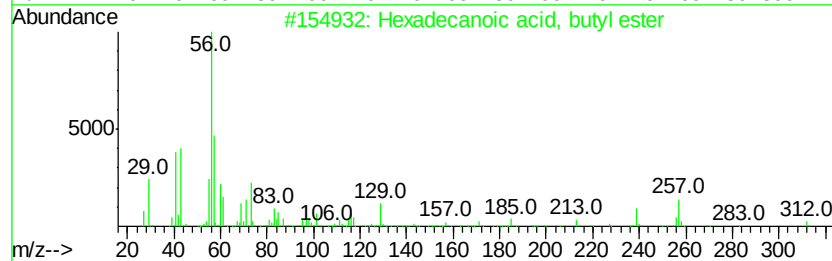
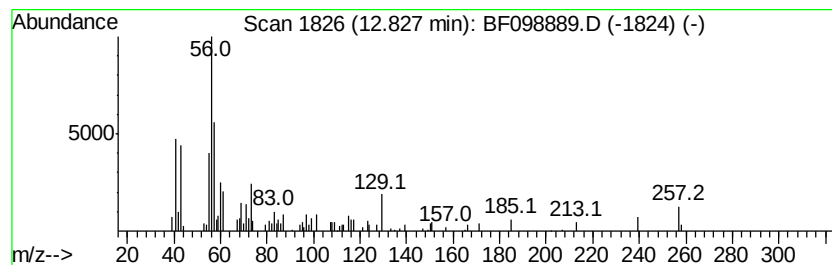
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	3.01 ng	142587	Chrysene-d12	14.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
4		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	27
5		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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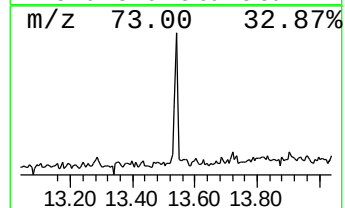
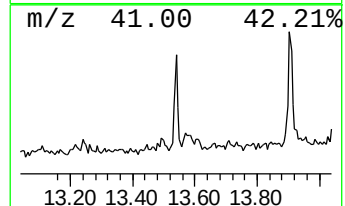
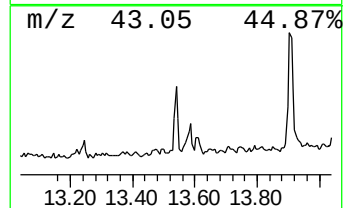
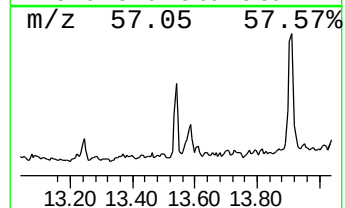
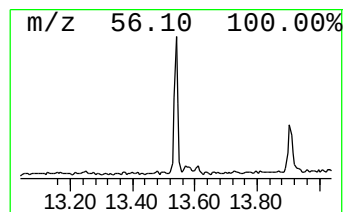
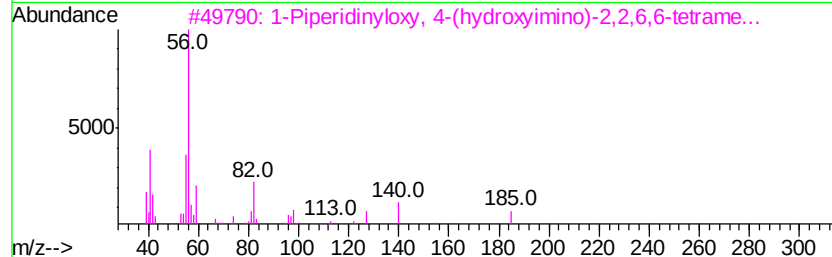
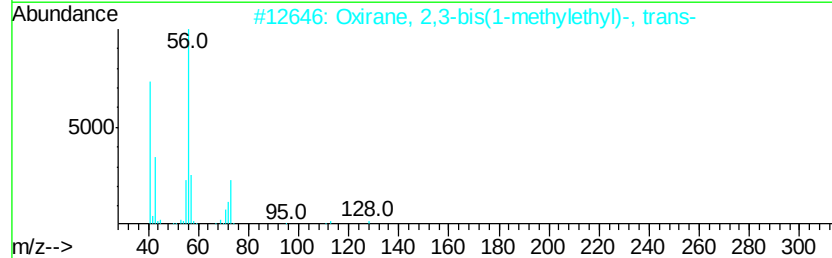
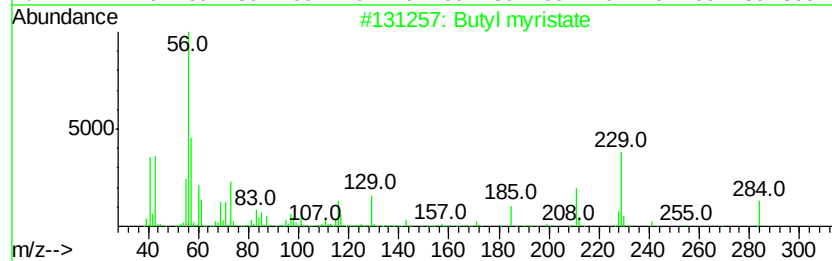
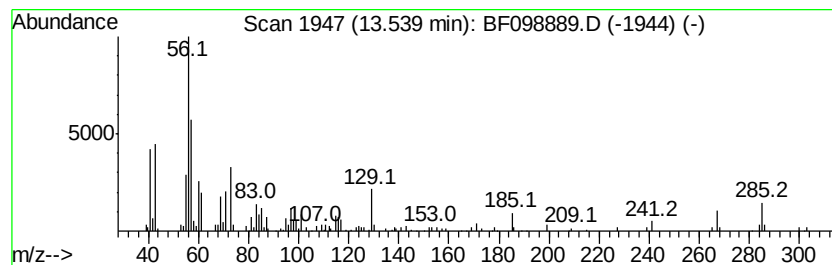
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Butyl myristate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.54	2.14 ng	101314	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35
3	1-Piperidinylloxv, 4-(hydroximin...	185	C9H17N2O2	003229-75-2	35
4	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	32
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27



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ALS Vial : 25 Sample Multiplier: 1

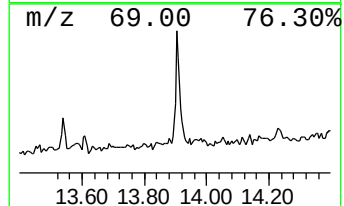
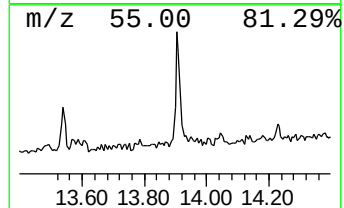
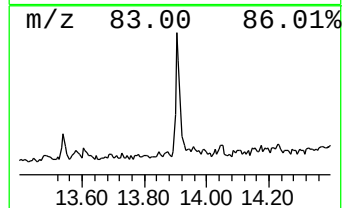
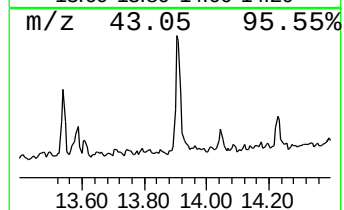
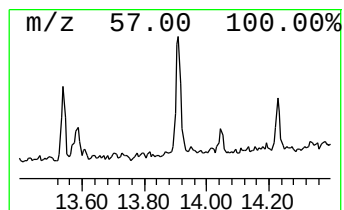
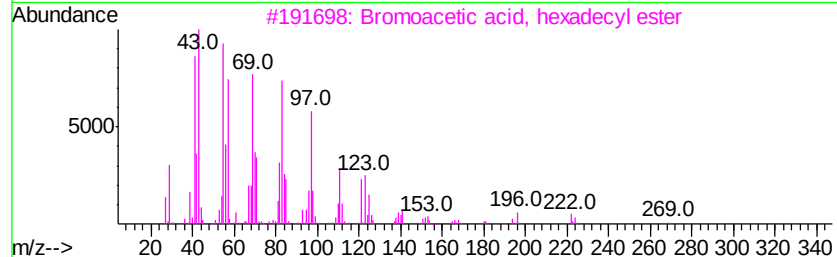
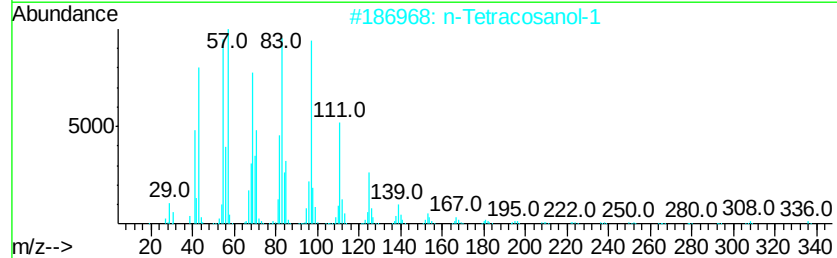
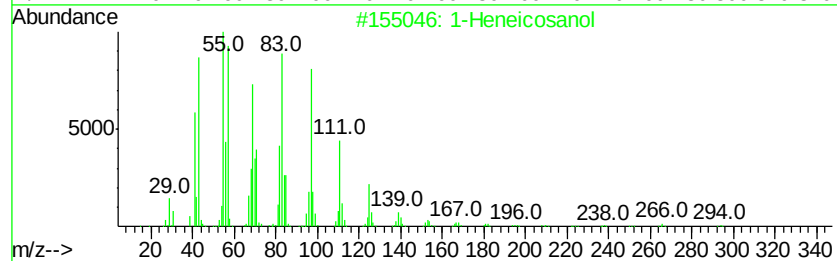
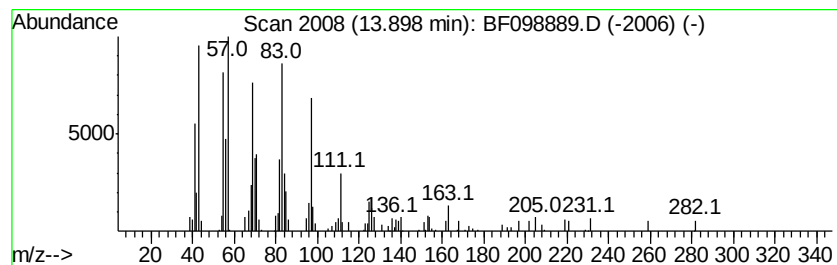
Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-B

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	4.07 ng	192761	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098889.D
Acq On : 28 Sep 2017 3:37
Operator : SJ/JU
Sample : I5396-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

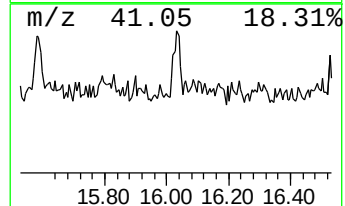
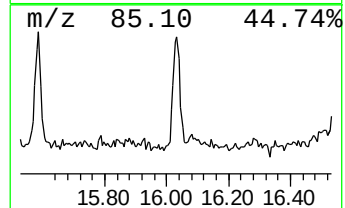
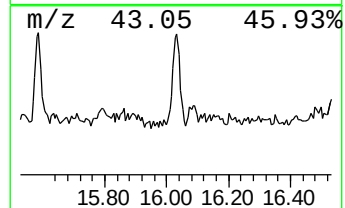
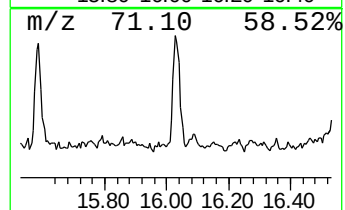
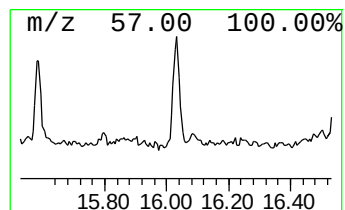
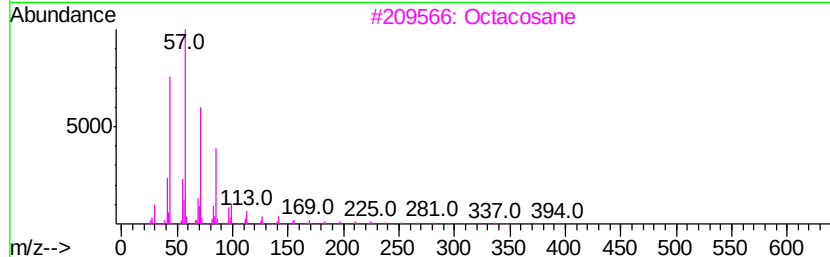
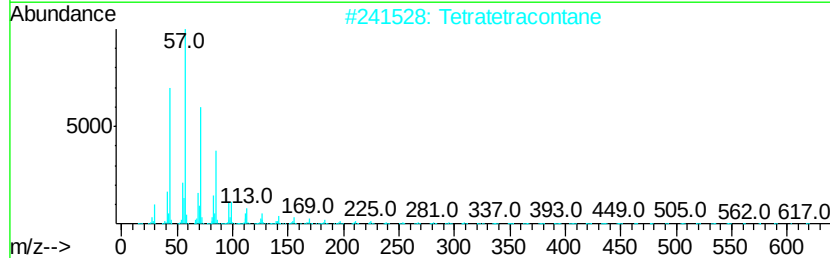
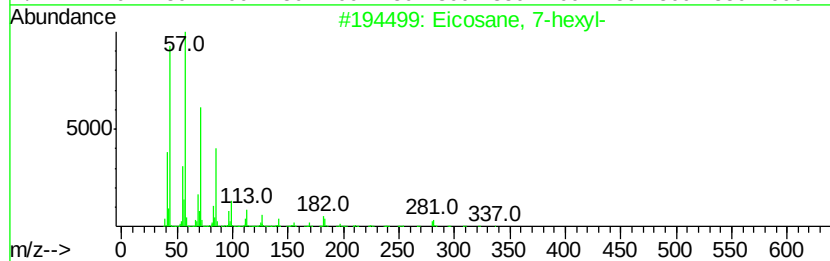
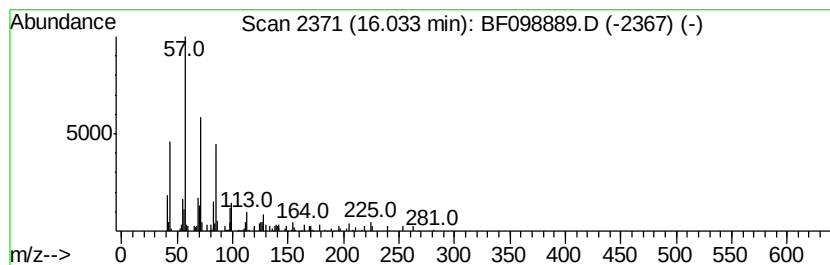
Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 7-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.53 ng	104659	Perylene-d12	15.57
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane, 7-hexyl-	366 C26H54	055333-99-8	87
2	Tetratetracontane	619 C44H90	007098-22-8	86
3	Octacosane	394 C28H58	000630-02-4	86
4	Pentacosane	352 C25H52	000629-99-2	86
5	10-Methylnonadecane	282 C20H42	056862-62-5	86



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098889.D
Acq On : 28 Sep 2017 3:37
Operator : SJ/JU
Sample : I5396-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-B

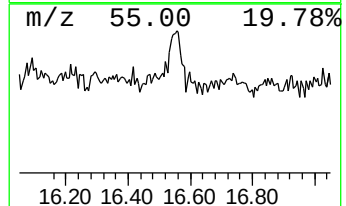
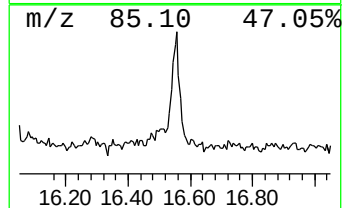
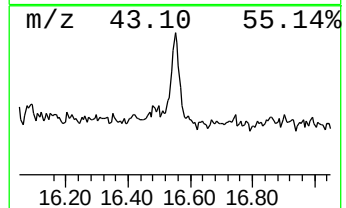
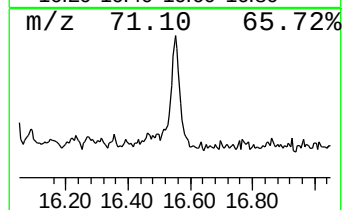
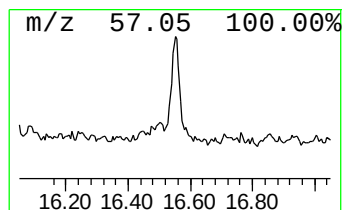
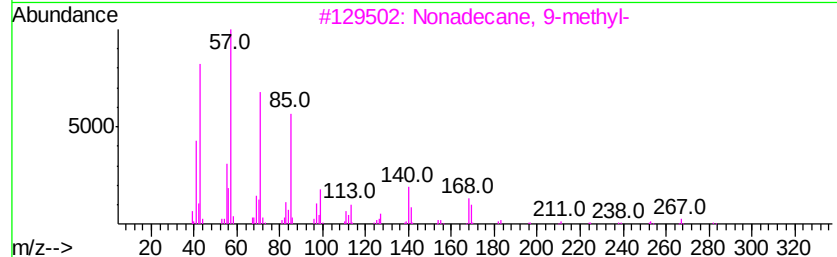
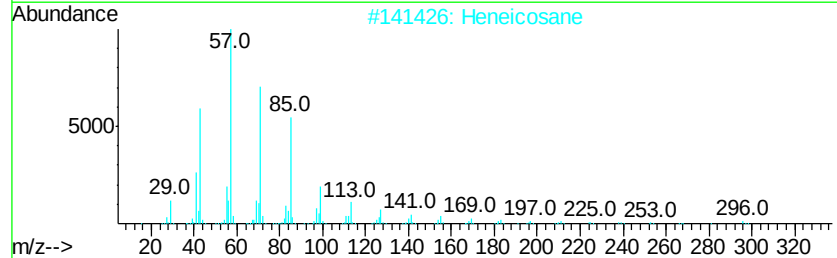
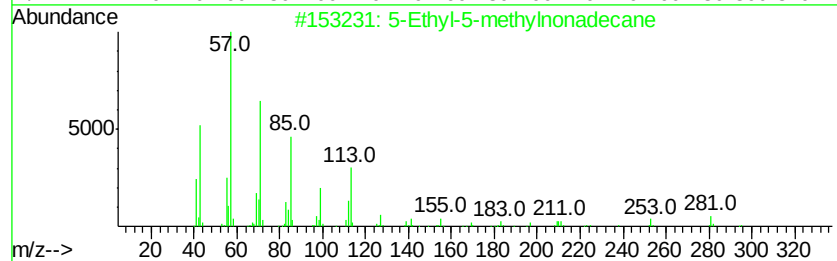
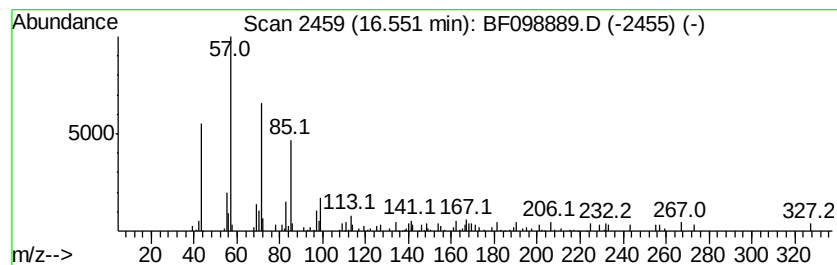
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Ethyl-5-methylnonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	2.80 ng	115687	Perylene-d12	15.57

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	72
2			Heneicosane	296	C21H44	000629-94-7	72
3			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	64
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5			Eicosane	282	C20H42	000112-95-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098889.D
Acq On : 28 Sep 2017 3:37
Operator : SJ/JU
Sample : I5396-02
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PAMT-COMP-B

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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
Butane, 2-methoxy...	2.23	2.8	ng	131529	1	6.92	949021	20.0
2-Pentanone, 4-hy...	5.15	15.3	ng	727991	1	6.92	949021	20.0
unknown6.69	6.69	76.3	ng	3619360	1	6.92	949021	20.0
Hexadecanoic acid...	12.83	3.0	ng	142587	5	14.08	947427	20.0
Butyl myristate	13.54	2.1	ng	101314	5	14.08	947427	20.0
1-Heneicosanol	13.90	4.1	ng	192761	5	14.08	947427	20.0
Eicosane, 7-hexyl-	16.03	2.5	ng	104659	6	15.57	827553	20.0
5-Ethyl-5-methyln...	16.55	2.8	ng	115687	6	15.57	827553	20.0