

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
 Data File : BF094956.D
 Acq On : 6 May 2017 12:25
 Operator : SJ/MA
 Sample : I2947-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-02-0-2.0

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-BF050217.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	5.042	524	528	547	rBV	129928	257658	10.61%	1.105%
2	5.666	630	634	660	rBV	1445051	2257333	92.98%	9.679%
3	7.260	900	905	921	rBV	1560299	2181912	89.88%	9.356%
4	7.383	921	926	938	rVB	1870222	2427656	100.00%	10.409%
5	7.719	980	983	996	rVB	423756	537401	22.14%	2.304%
6	7.960	1019	1024	1042	rBV	1598216	1841033	75.84%	7.894%
7	8.619	1131	1136	1152	rBV	992980	1338959	55.15%	5.741%
8	9.742	1322	1327	1340	rBV	505452	707301	29.14%	3.033%
9	11.513	1623	1628	1640	rBV	1917384	2360504	97.23%	10.122%
10	11.736	1661	1666	1672	rVB	37040	44788	1.84%	0.192%
11	12.207	1742	1746	1753	rBV	250989	312515	12.87%	1.340%
12	12.571	1803	1808	1812	rBV2	602861	835102	34.40%	3.581%
13	13.412	1947	1951	1957	rBV	98162	106535	4.39%	0.457%
14	13.777	2007	2013	2016	rBV2	23807	36117	1.49%	0.155%
15	13.865	2023	2028	2040	rBV	1026656	1503147	61.92%	6.445%
16	14.189	2078	2083	2085	rBV	89282	116083	4.78%	0.498%
17	14.918	2203	2207	2211	rBV2	59186	69940	2.88%	0.300%
18	14.971	2211	2216	2227	rBV	619909	877997	36.17%	3.765%
19	15.942	2378	2381	2386	rBV2	168075	225549	9.29%	0.967%
20	16.759	2518	2520	2537	rVB3	75971	166360	6.85%	0.713%
21	17.024	2562	2565	2569	rBV4	38198	49754	2.05%	0.213%
22	17.059	2569	2571	2579	rVB	40260	48595	2.00%	0.208%
23	17.295	2606	2611	2619	rVB	1766636	2201974	90.70%	9.442%
24	17.683	2674	2677	2681	rVB	24522	25893	1.07%	0.111%
25	18.547	2816	2824	2826	rBV	35836	50083	2.06%	0.215%
26	18.589	2826	2831	2835	rVV6	48796	124743	5.14%	0.535%
27	18.642	2835	2840	2853	rVB	523166	797639	32.86%	3.420%
28	18.947	2887	2892	2899	rBV5	18093	26983	1.11%	0.116%
29	19.330	2953	2957	2962	rVB	82668	93994	3.87%	0.403%
30	19.406	2964	2970	2974	rBV7	17186	44251	1.82%	0.190%
31	19.853	3042	3046	3050	rVB	26270	29257	1.21%	0.125%
32	20.053	3075	3080	3088	rBV	454296	525280	21.64%	2.252%
33	20.306	3119	3123	3136	rBV	372278	525605	21.65%	2.254%
34	20.571	3164	3168	3173	rVB3	39732	46181	1.90%	0.198%

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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	20.777	3198	3203	3210	rVB	113169	157488	6.49%	0.675%
36	20.877	3214	3220	3222	rBV6	17605	34211	1.41%	0.147%
37	21.441	3312	3316	3324	rVB2	22029	35690	1.47%	0.153%
38	21.694	3354	3359	3366	rVB4	25279	45403	1.87%	0.195%
39	21.835	3379	3383	3390	rVB8	14805	27827	1.15%	0.119%
40	22.094	3420	3427	3434	rBV10	15564	43786	1.80%	0.188%
41	22.388	3466	3477	3484	rBV10	28348	95948	3.95%	0.411%
42	22.771	3534	3542	3544	rBV7	19257	45670	1.88%	0.196%
43	23.741	3700	3707	3717	rVB10	17707	41417	1.71%	0.178%

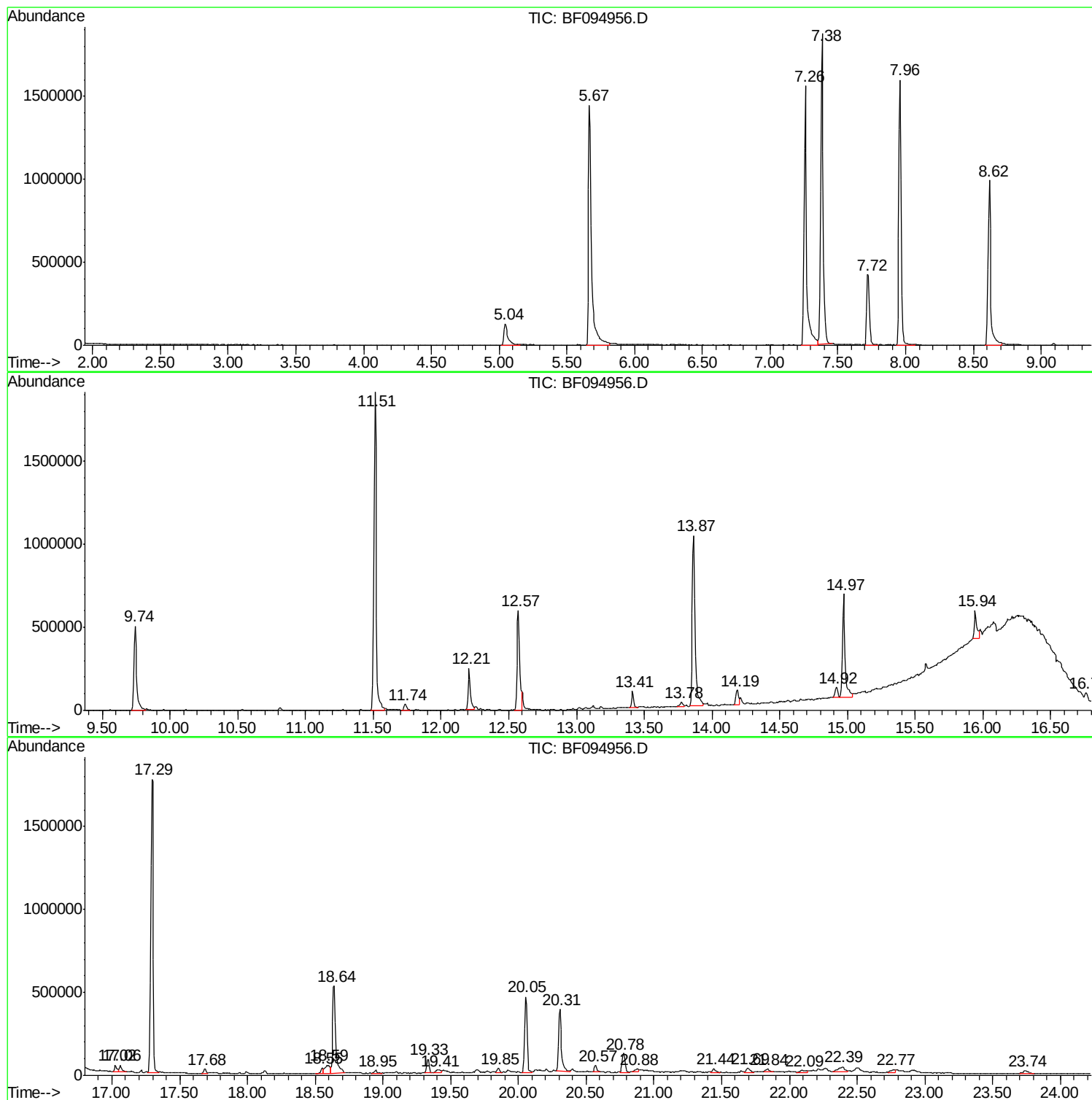
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SB-02-0-2.0

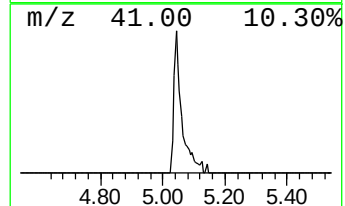
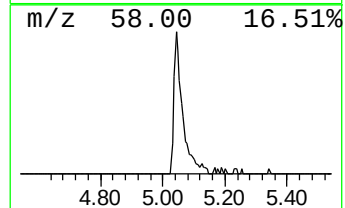
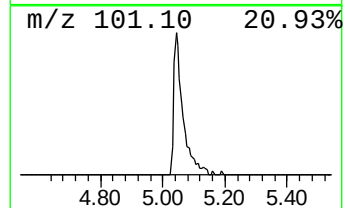
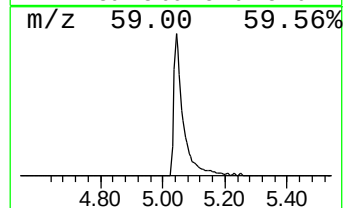
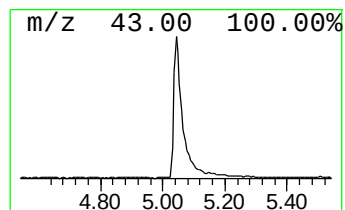
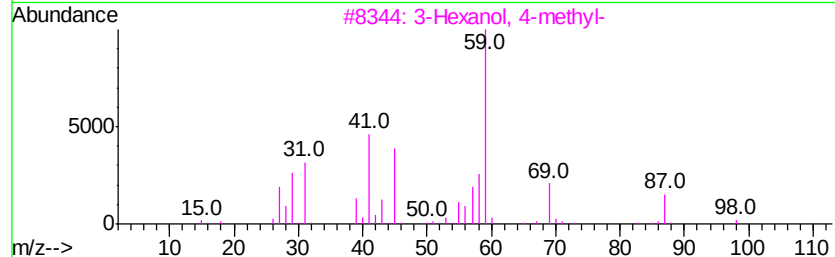
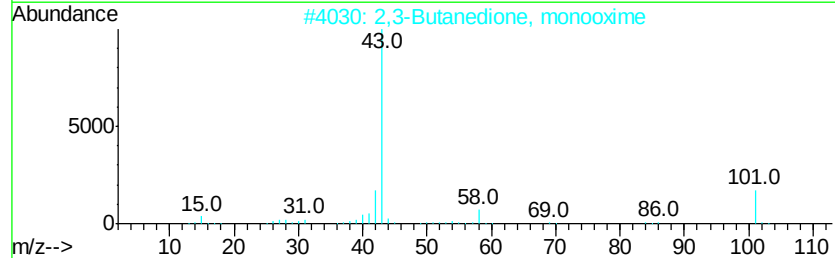
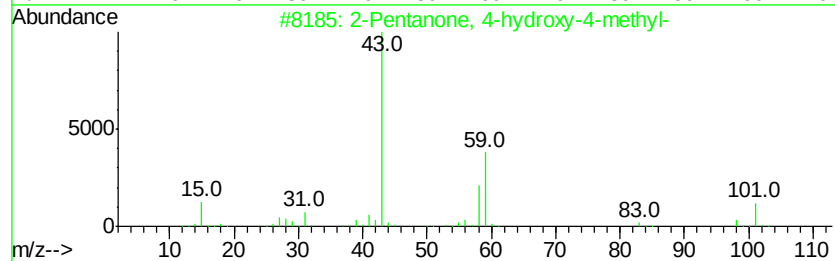
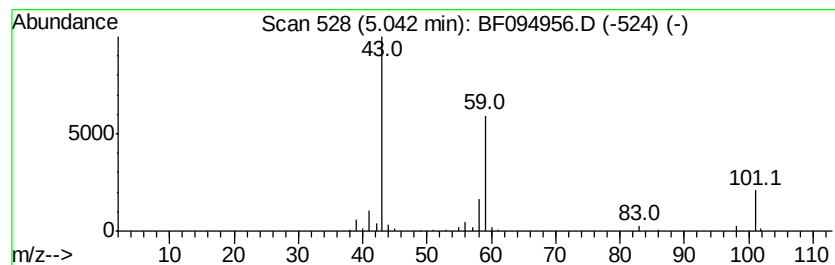
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	9.59 ng	257658	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	25
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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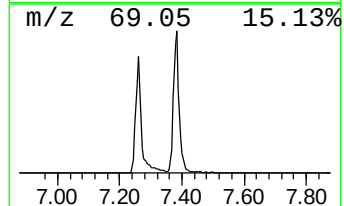
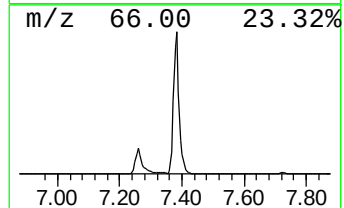
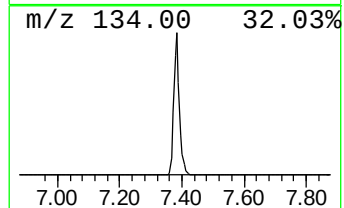
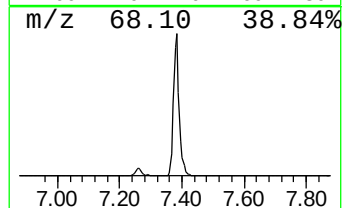
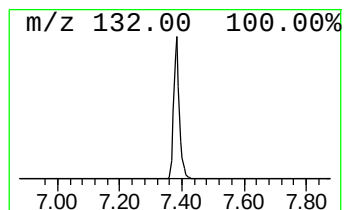
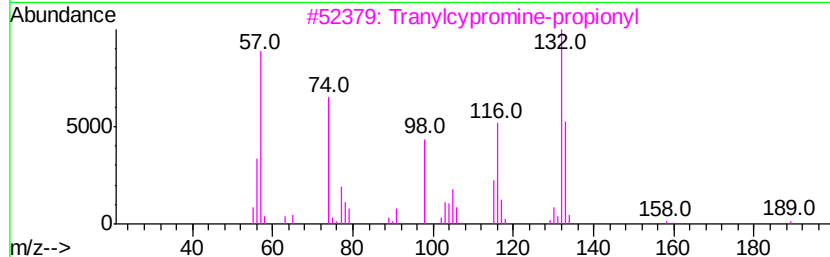
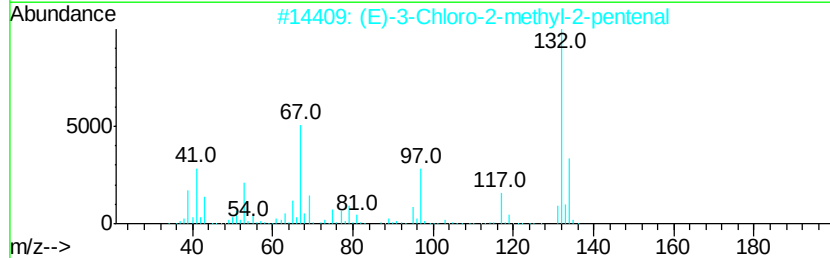
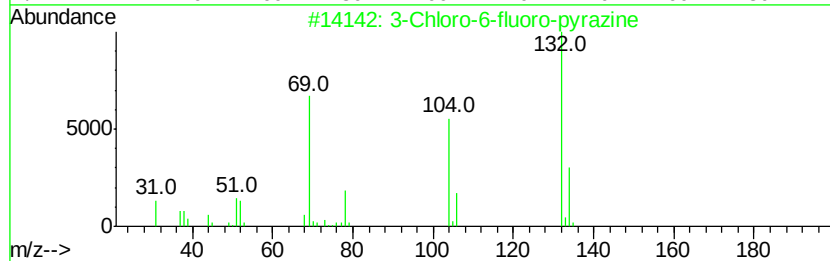
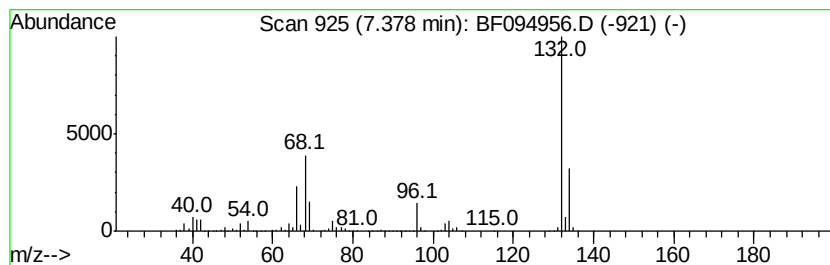
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	90.35 ng	2427660	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Xenon	132	Xe	007440-63-3	9



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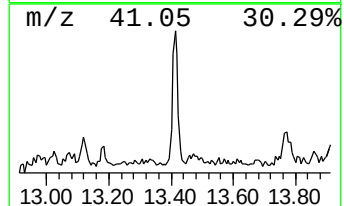
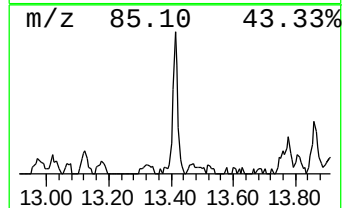
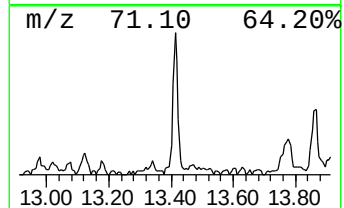
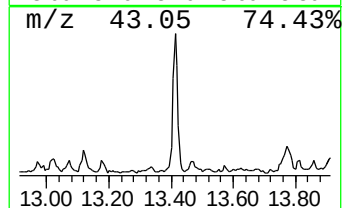
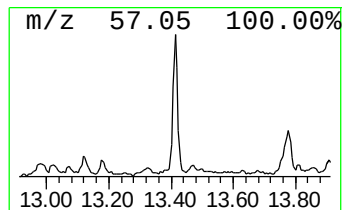
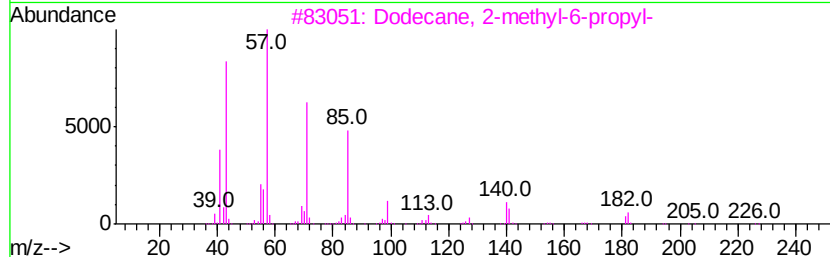
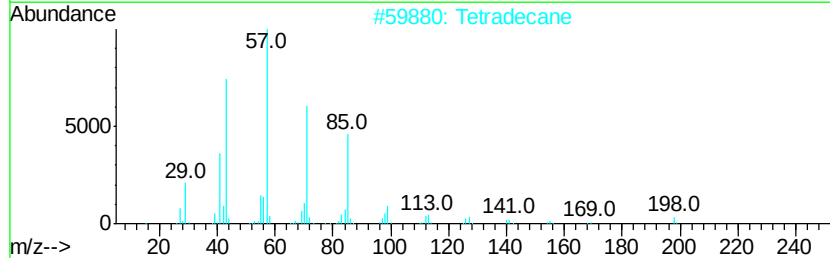
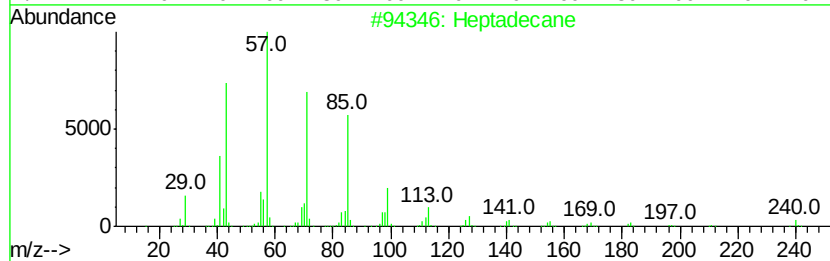
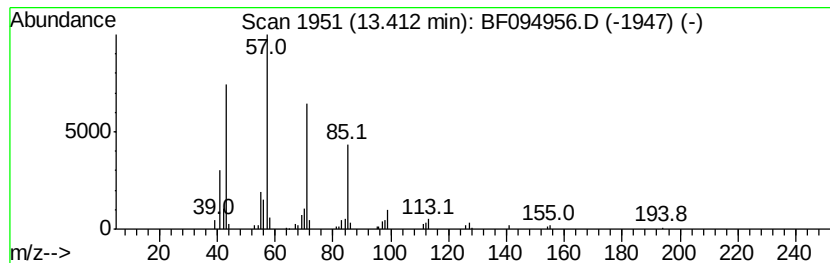
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.41	2.55 ng	106535	Acenaphthene-d10	12.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
4	Hexadecane	226	C16H34	000544-76-3	80
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72



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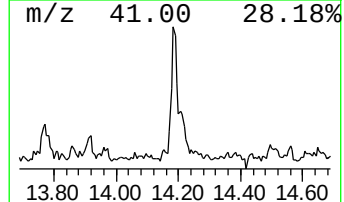
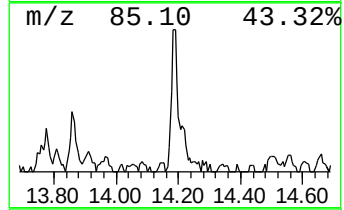
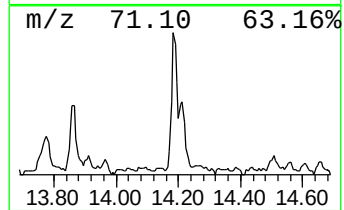
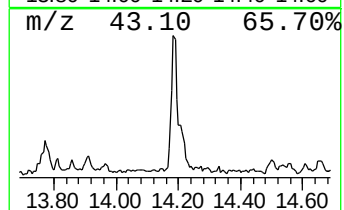
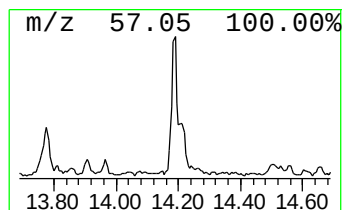
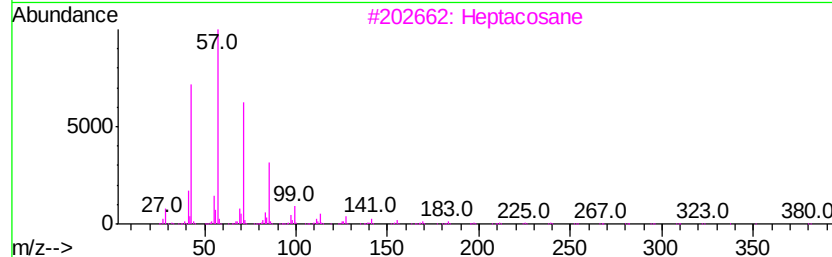
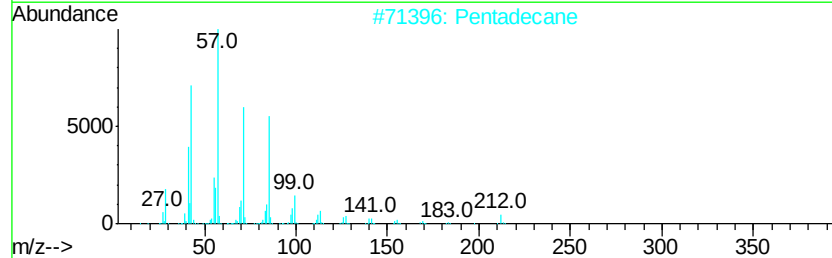
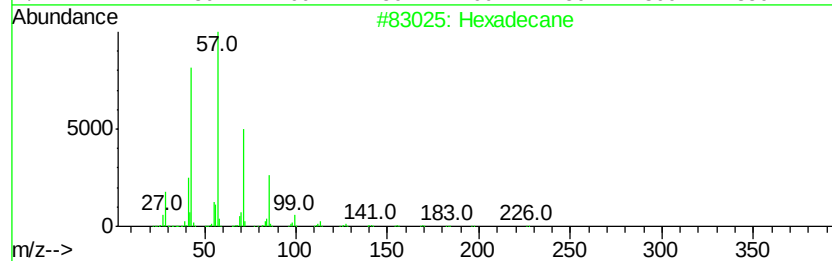
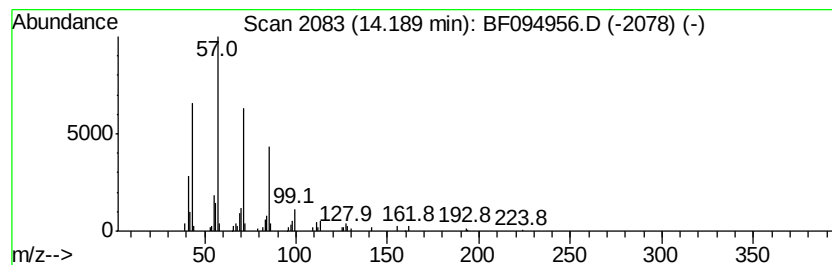
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.19	2.64 ng	116083	Phenanthrene-d10	14.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	90
2		Pentadecane	212	C15H32	000629-62-9	90
3		Heptacosane	380	C27H56	000593-49-7	86
4		Tetradecane	198	C14H30	000629-59-4	86
5		Tridecane	184	C13H28	000629-50-5	86



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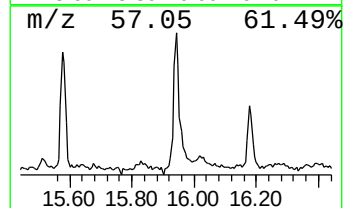
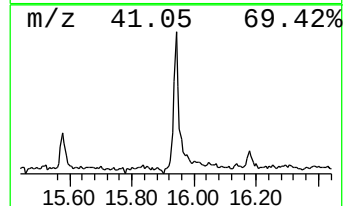
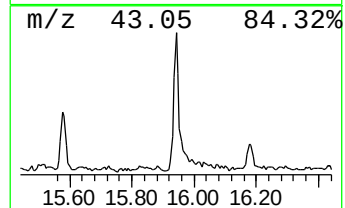
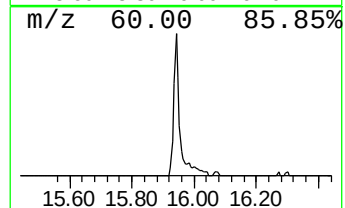
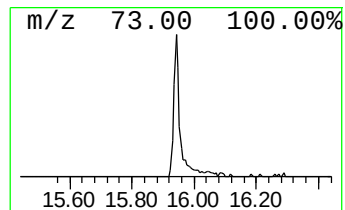
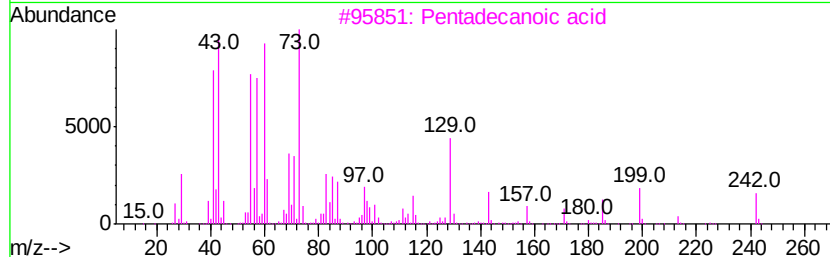
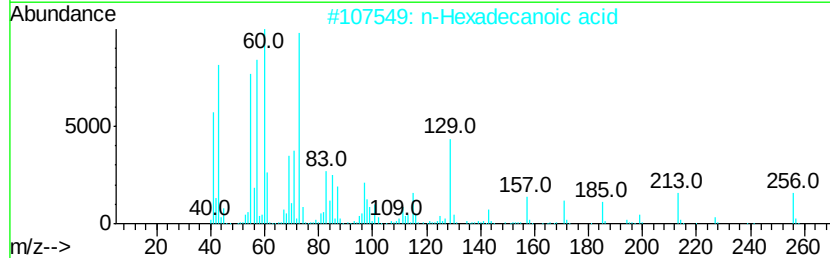
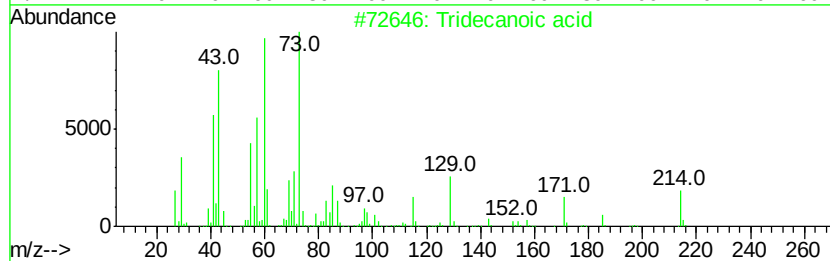
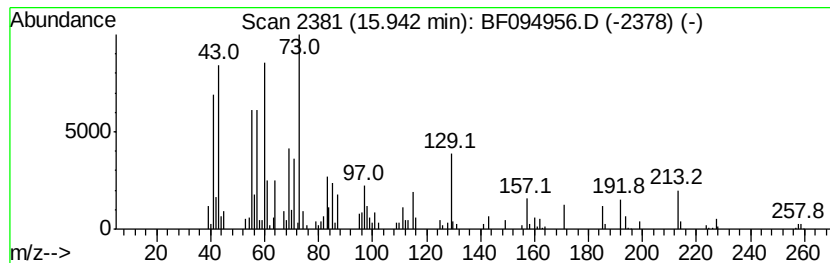
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Peak Number 6 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.94	5.14 ng	225549	Phenanthrene-d10	14.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094956.D
Acq On : 6 May 2017 12:25
Operator : SJ/MA
Sample : I2947-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
SB-02-0-2.0

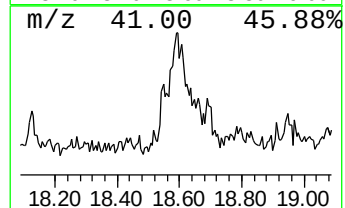
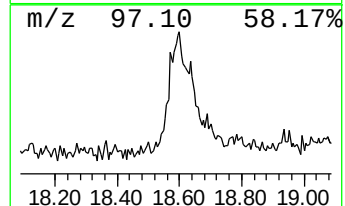
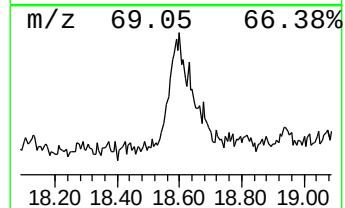
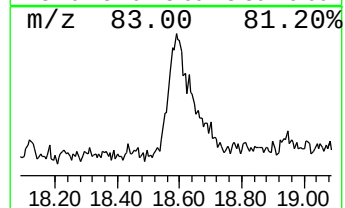
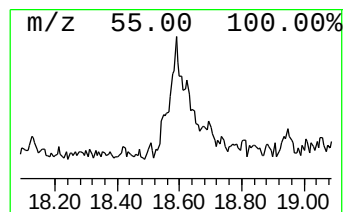
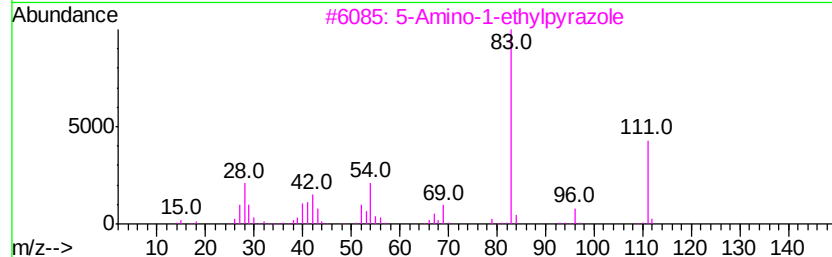
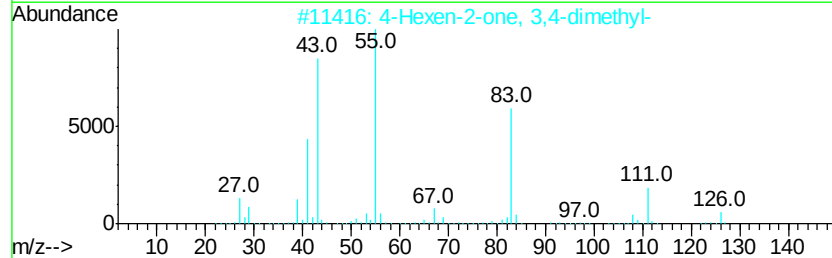
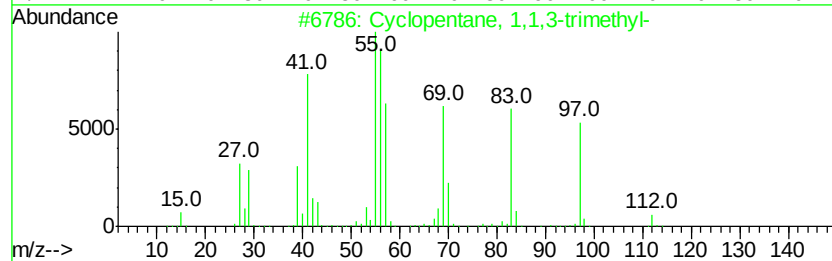
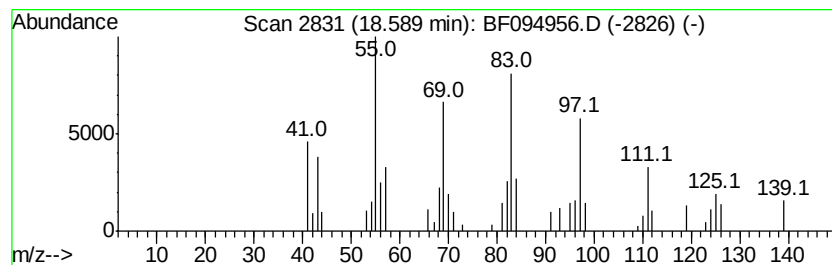
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.59 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.59	3.13 ng	124743	Chrysene-d12	18.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	43
2	4-Hexen-2-one, 3,4-dimethyl-	126	C8H14O	053252-21-4	38
3	5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	35
4	2,4-Pentadien-1-ol, 3-ethyl-, (2Z)-	112	C7H12O	1000142-17-6	35
5	2H-Pyrazole, 3-amino-2-isopropyl-	125	C6H11N3	1000315-90-7	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094956.D
Acq On : 6 May 2017 12:25
Operator : SJ/MA
Sample : I2947-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

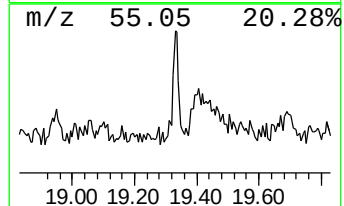
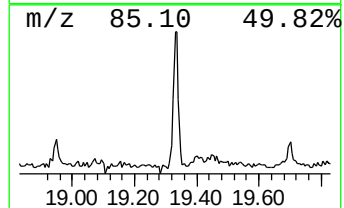
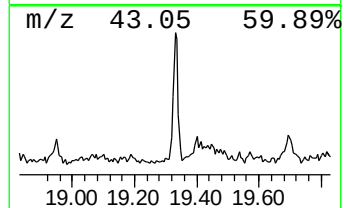
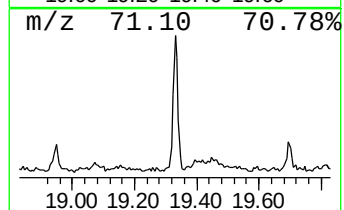
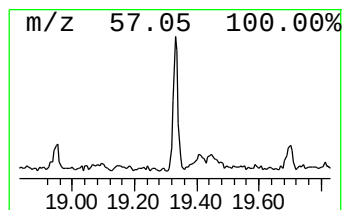
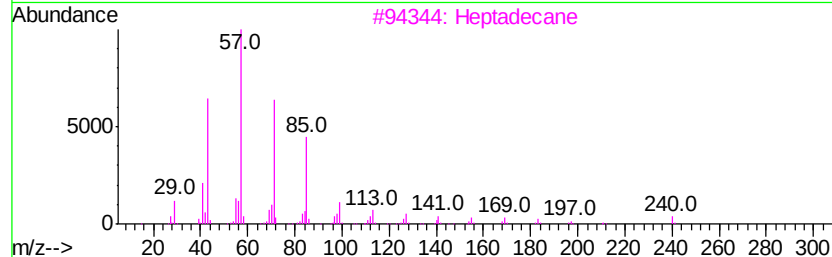
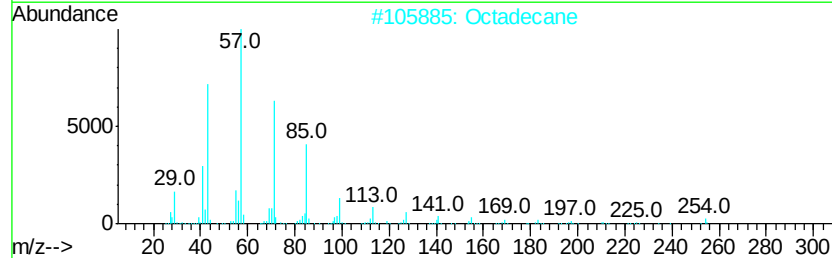
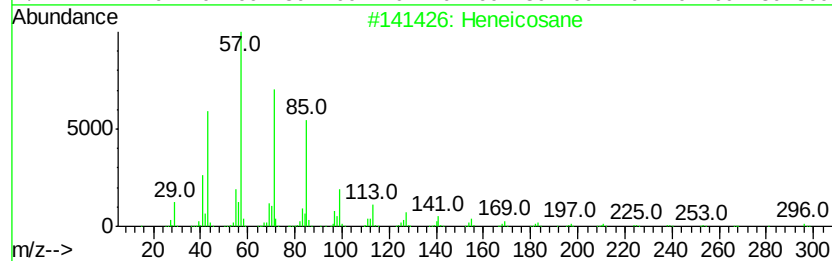
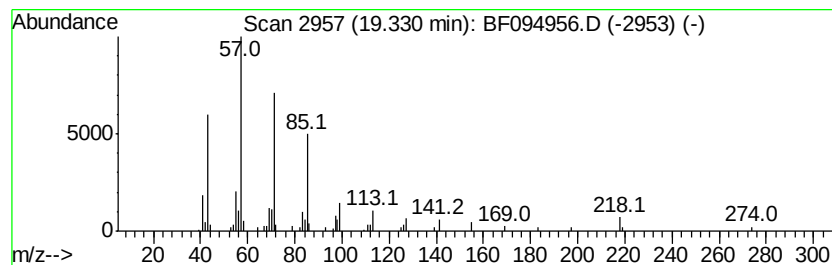
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	2.36 ng	93994	Chrysene-d12	18.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	91
2	Octadecane		254	C18H38	000593-45-3	91
3	Heptadecane		240	C17H36	000629-78-7	91
4	Docosane		310	C22H46	000629-97-0	91
5	Hexadecane		226	C16H34	000544-76-3	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF050617\
Data File : BF094956.D
Acq On : 6 May 2017 12:25
Operator : SJ/MA
Sample : I2947-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

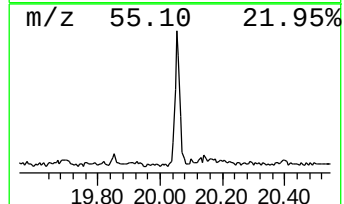
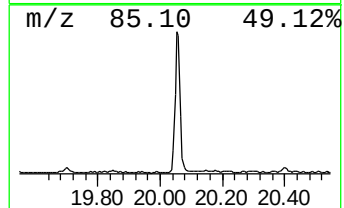
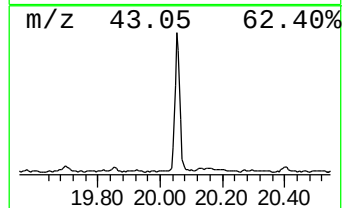
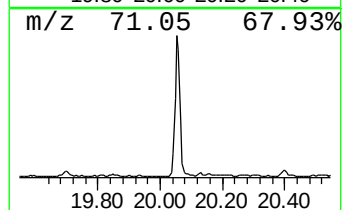
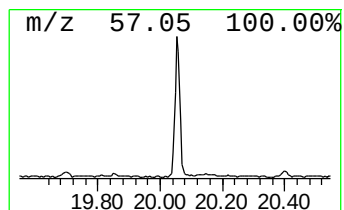
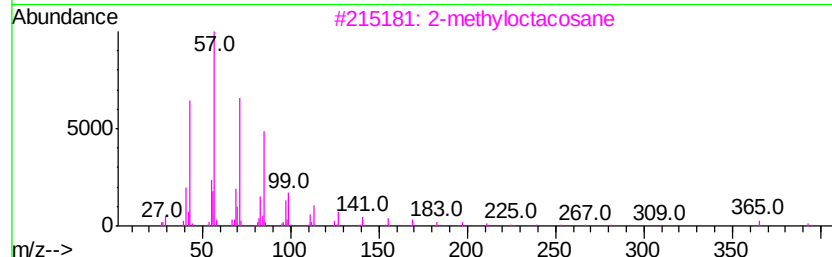
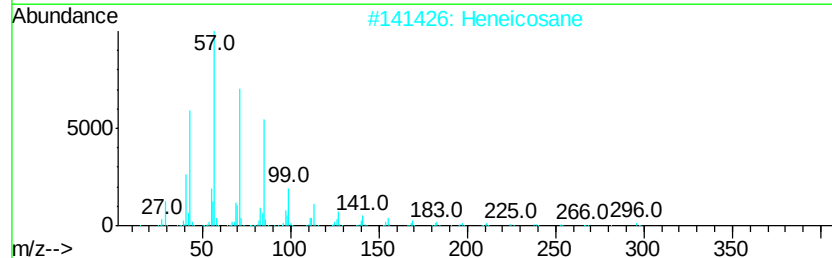
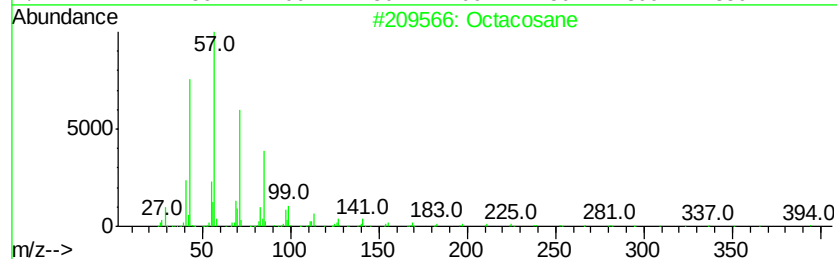
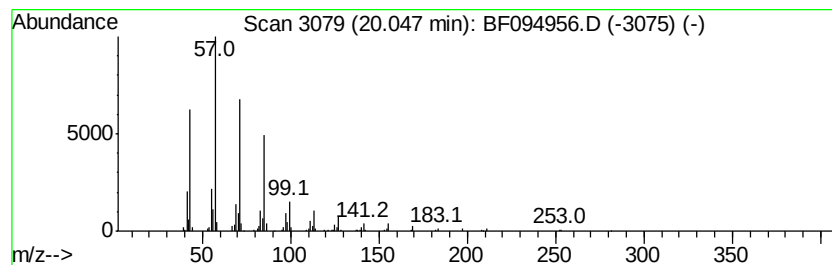
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.05	19.99 ng	525280	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Tetratetracontane	619	C44H90	007098-22-8	90
5		Heptadecane	240	C17H36	000629-78-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094956.D
Acq On : 6 May 2017 12:25
Operator : SJ/MA
Sample : I2947-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

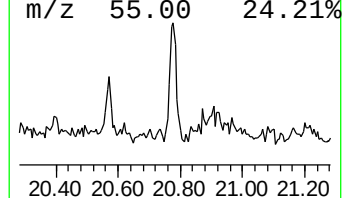
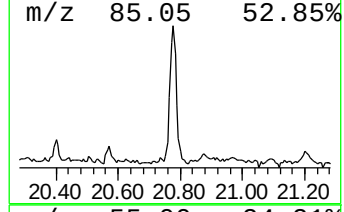
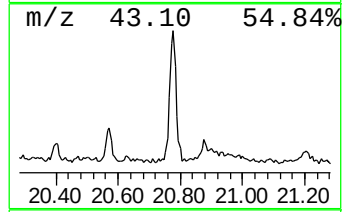
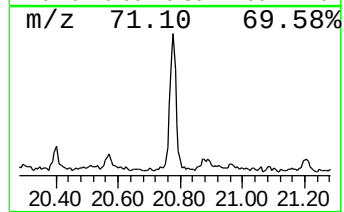
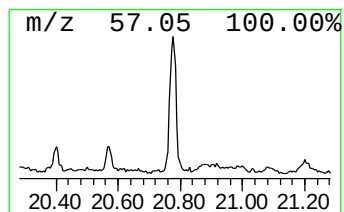
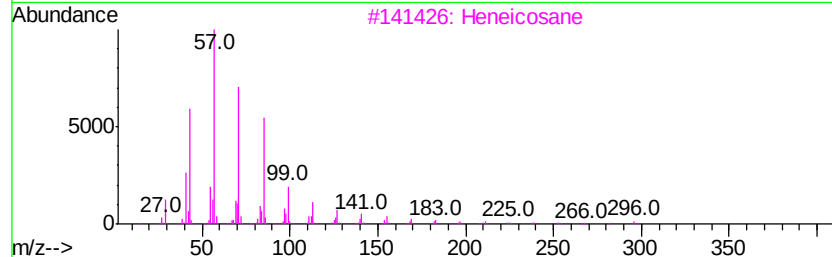
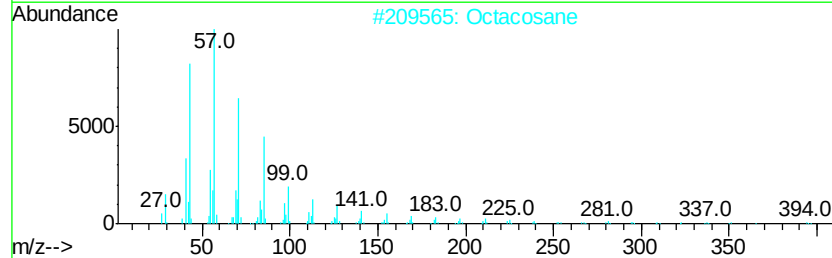
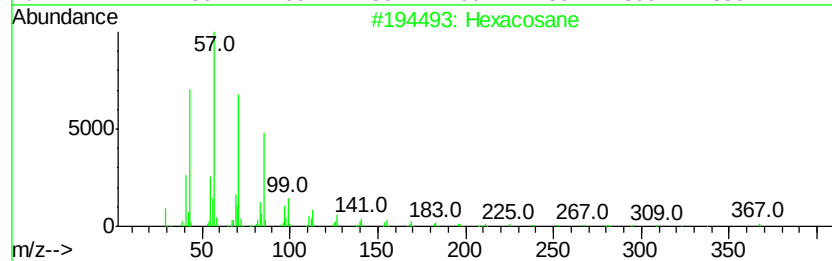
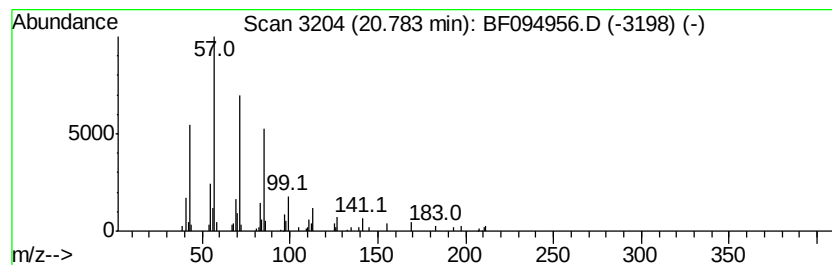
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.78	5.99 ng	157488	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Heptacosane	380	C27H56	000593-49-7	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
Data File : BF094956.D
Acq On : 6 May 2017 12:25
Operator : SJ/MA
Sample : I2947-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

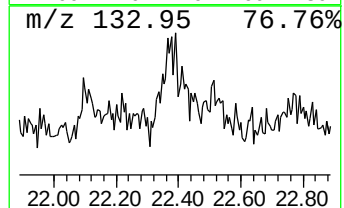
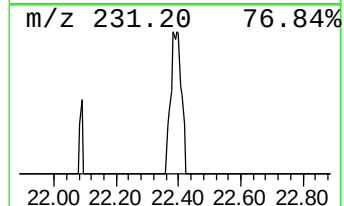
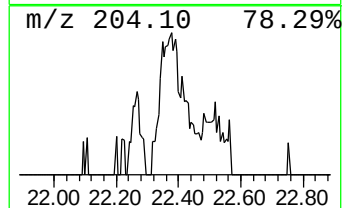
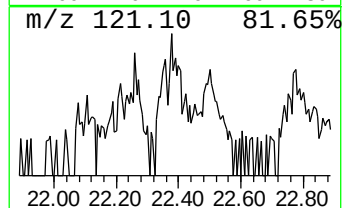
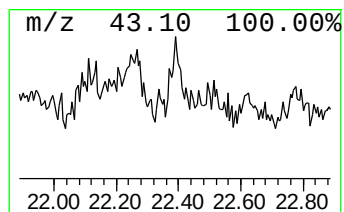
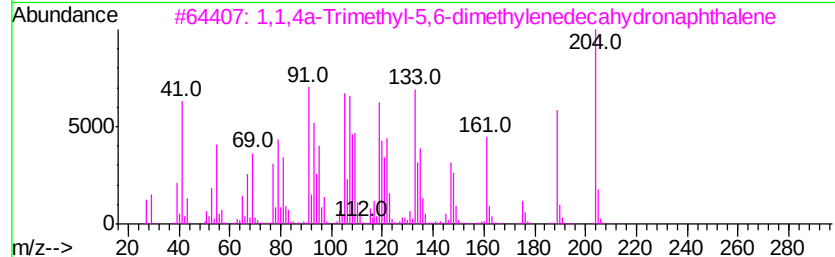
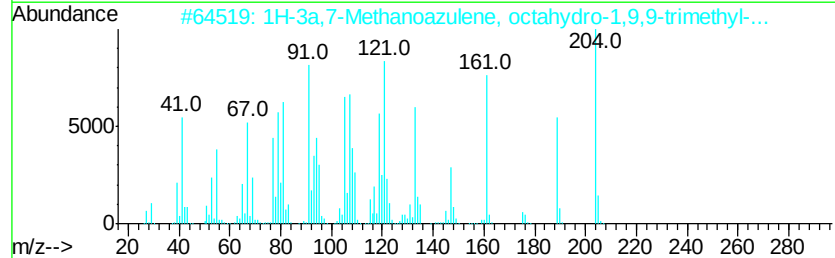
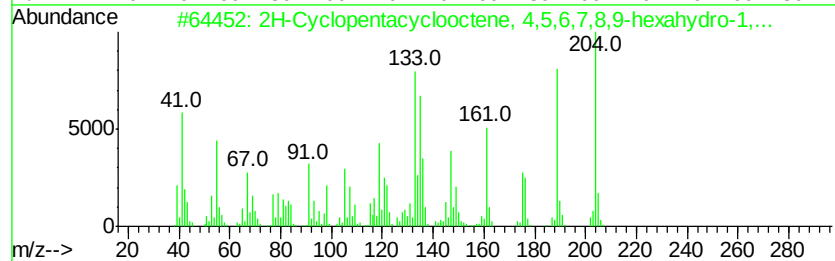
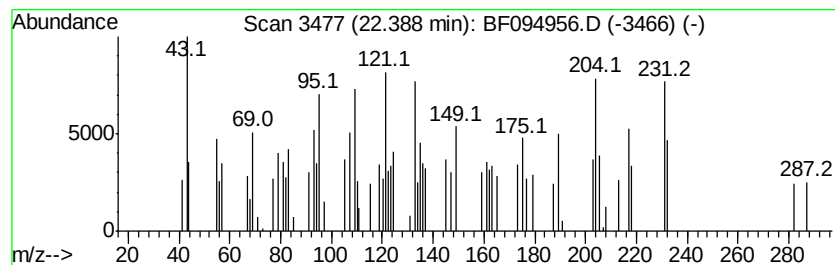
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2H-Cyclopentacyclooctene, 4... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	3.65 ng	95948	Perylene-d12	20.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	49
2		1H-3a,7-Methanoazulene, octahydr...	204	C15H24	000508-55-4	38
3		1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	25
4		2-Benzothiazolamine, N-(1-methyl...	231	C12H13N3S	084859-07-4	25
5		1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050617\
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Acq On : 6 May 2017 12:25
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Sample : I2947-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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
2-Pentanone, 4-hy...	5.04	9.6 ng		257658	1	7.72	537401	20.0
unknown7.38	7.38	90.3 ng		2427660	1	7.72	537401	20.0
Heptadecane	13.41	2.5 ng		106535	3	12.57	835102	20.0
Hexadecane	14.19	2.6 ng		116083	4	14.97	877997	20.0
Tridecanoic acid	15.94	5.1 ng		225549	4	14.97	877997	20.0
unknown18.59	18.59	3.1 ng		124743	5	18.64	797639	20.0
Heneicosane	19.33	2.4 ng		93994	5	18.64	797639	20.0
Octacosane	20.05	20.0 ng		525280	6	20.31	525605	20.0
Hexacosane	20.78	6.0 ng		157488	6	20.31	525605	20.0
2H-Cyclopentacycl...	22.39	3.6 ng		95948	6	20.31	525605	20.0