

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
 Data File : BF098860.D
 Acq On : 27 Sep 2017 13:50
 Operator : SJ/JU
 Sample : I5434-12
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 UT5400533

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	2.240	20	26	32	rVB	109840	140304	3.71%	0.397%
2	5.151	516	521	532	rVB	567941	793128	20.95%	2.245%
3	5.539	581	587	590	rBV	3469762	3584392	94.66%	10.145%
4	6.539	751	757	760	rBV	3257763	3786506	100.00%	10.717%
5	6.686	777	782	785	rBV	3686149	3728967	98.48%	10.554%
6	6.916	817	821	824	rVB	992178	874599	23.10%	2.475%
7	7.069	843	847	851	rBV	2738061	2373586	62.69%	6.718%
8	7.475	910	916	919	rBV	2271581	2338888	61.77%	6.620%
9	8.192	1034	1038	1042	rBV	1295703	1200318	31.70%	3.397%
10	9.269	1216	1221	1224	rBV	3932497	3757437	99.23%	10.634%
11	9.657	1283	1287	1291	rBV	676586	544519	14.38%	1.541%
12	9.951	1333	1337	1341	rVB	1549507	1314526	34.72%	3.720%
13	10.374	1406	1409	1412	rVB	72732	62493	1.65%	0.177%
14	10.739	1464	1471	1474	rBV	2306293	2261636	59.73%	6.401%
15	10.845	1486	1489	1494	rBV	97224	90226	2.38%	0.255%
16	11.292	1562	1565	1568	rBV	50734	37906	1.00%	0.107%
17	11.439	1586	1590	1593	rBV	1516598	1288875	34.04%	3.648%
18	11.951	1674	1677	1681	rBV	86838	80677	2.13%	0.228%
19	13.021	1854	1859	1863	rBV	3301539	3438303	90.80%	9.731%
20	13.568	1949	1952	1957	rBV	41682	58056	1.53%	0.164%
21	13.904	2006	2009	2013	rBV	277689	264063	6.97%	0.747%
22	14.074	2034	2038	2042	rBV	979393	841702	22.23%	2.382%
23	14.227	2057	2064	2069	rBV3	22677	38329	1.01%	0.108%
24	14.539	2112	2117	2123	rBV	112341	149249	3.94%	0.422%
25	14.827	2162	2166	2171	rBV2	122151	152993	4.04%	0.433%
26	14.992	2191	2194	2200	rVB	61041	65434	1.73%	0.185%
27	15.192	2223	2228	2230	rBV	186991	210577	5.56%	0.596%
28	15.215	2230	2232	2239	rVB	54974	64976	1.72%	0.184%
29	15.568	2286	2292	2298	rBV	577338	768308	20.29%	2.174%
30	15.786	2325	2329	2334	rBV	65898	87172	2.30%	0.247%
31	16.027	2365	2370	2375	rBV2	75064	109346	2.89%	0.309%
32	16.080	2375	2379	2385	rVB6	38904	65520	1.73%	0.185%
33	16.545	2454	2458	2465	rVB4	24485	44244	1.17%	0.125%
34	16.850	2504	2510	2517	rBV3	59054	109804	2.90%	0.311%

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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

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Peak separation: 5

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35	17.080	2546	2549	2556	rVB9	25023	43898	1.16%	0.124%
36	17.156	2557	2562	2569	rVB3	29626	61497	1.62%	0.174%
37	17.245	2572	2577	2585	rBV7	21122	48821	1.29%	0.138%
38	17.674	2641	2650	2660	rBV6	116354	310637	8.20%	0.879%
39	18.509	2785	2792	2796	rBV8	39639	102228	2.70%	0.289%
40	18.727	2827	2829	2837	rVB7	20072	38495	1.02%	0.109%

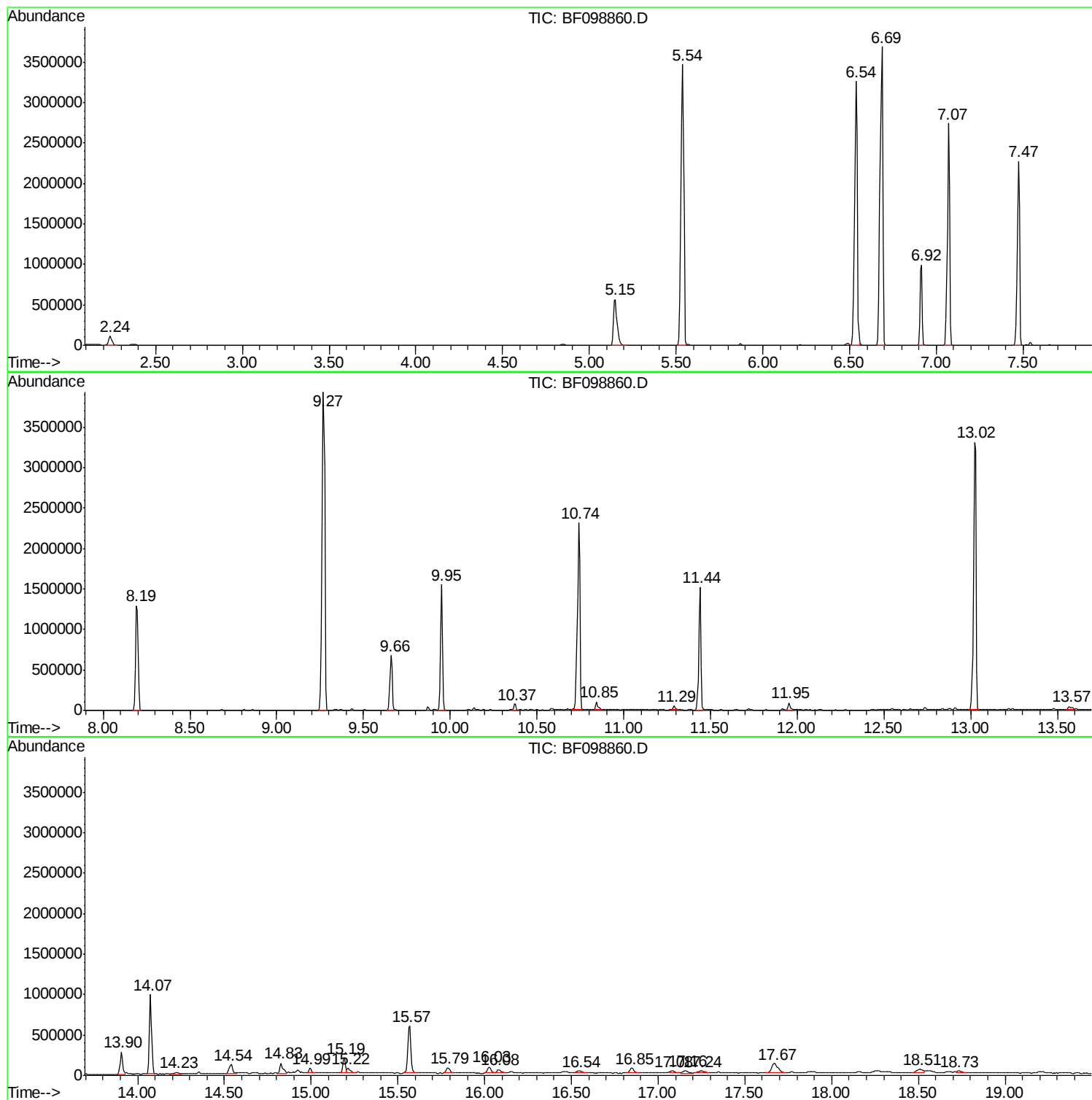
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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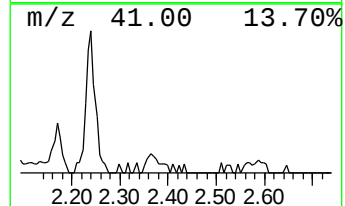
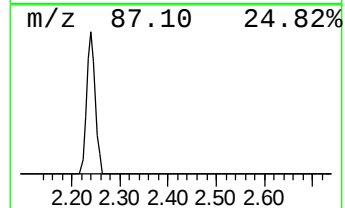
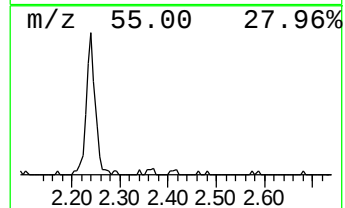
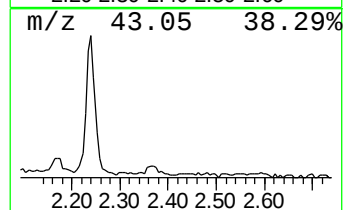
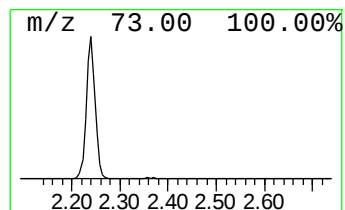
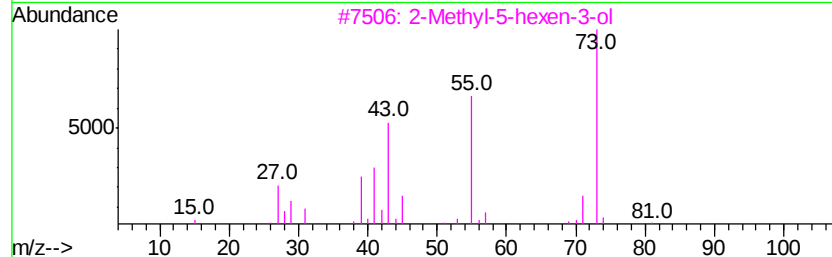
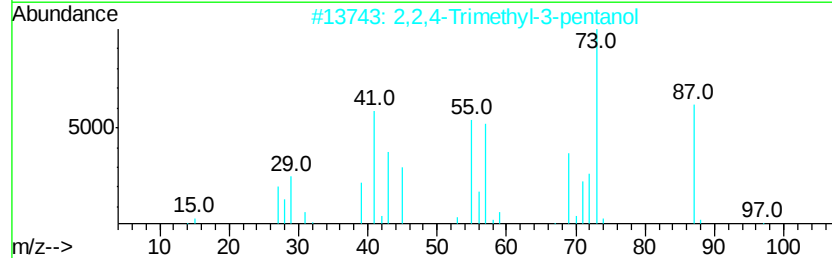
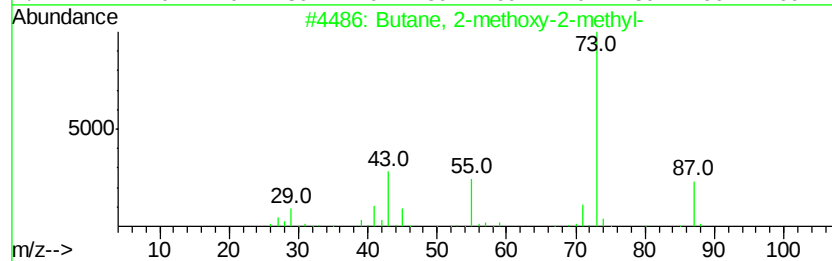
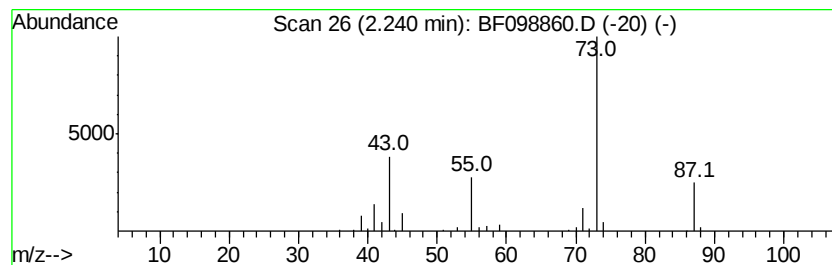
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	3.21 ng	140304	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	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4		Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16



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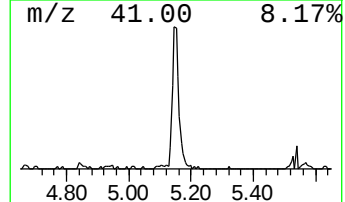
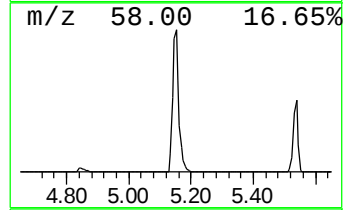
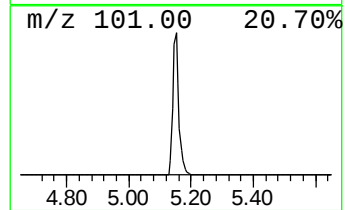
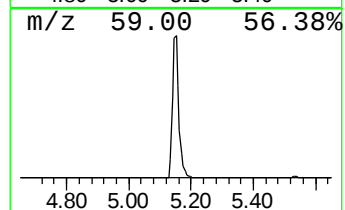
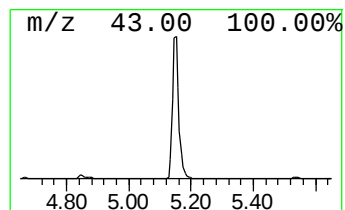
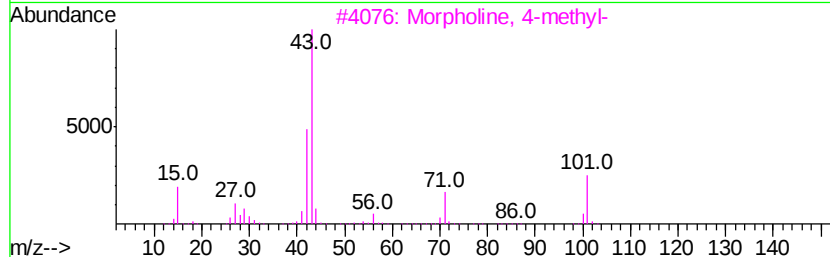
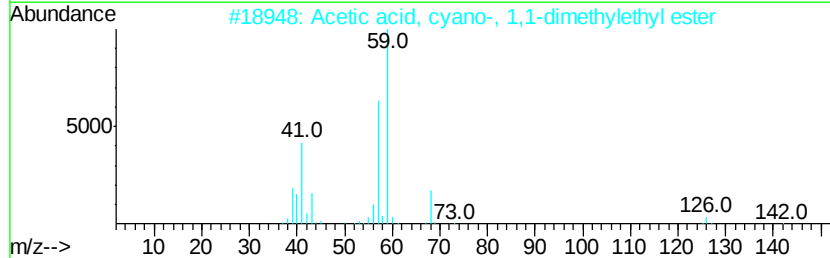
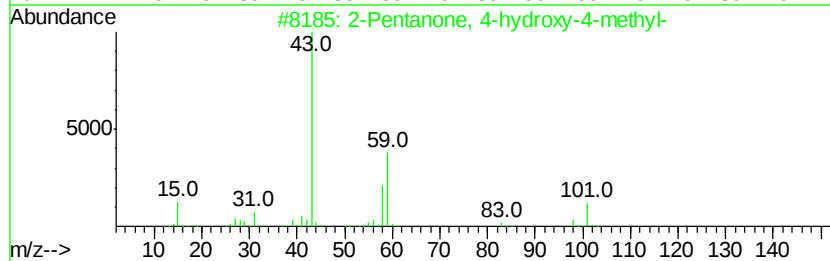
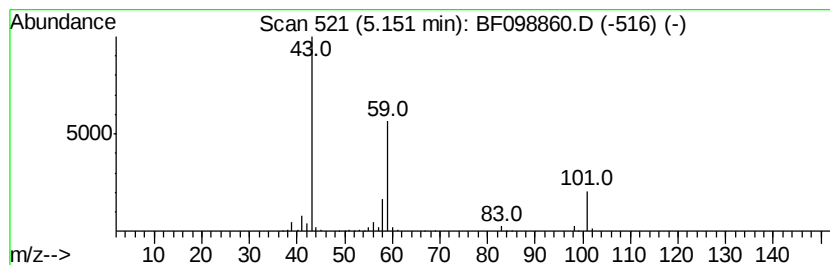
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	18.14 ng	793128	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	53
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		Acetone	58	C3H6O	000067-64-1	9



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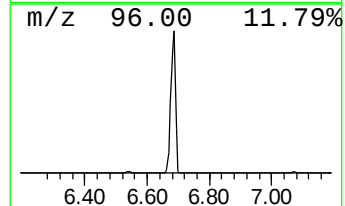
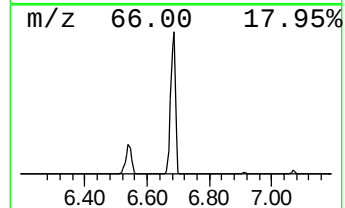
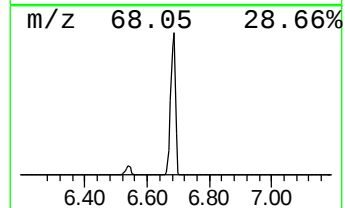
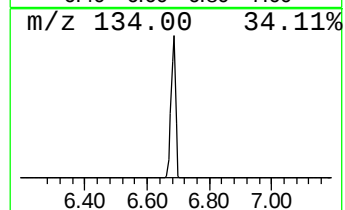
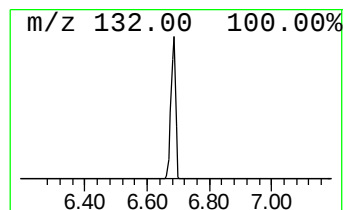
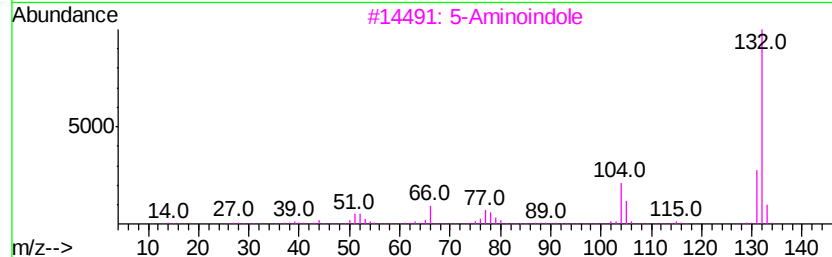
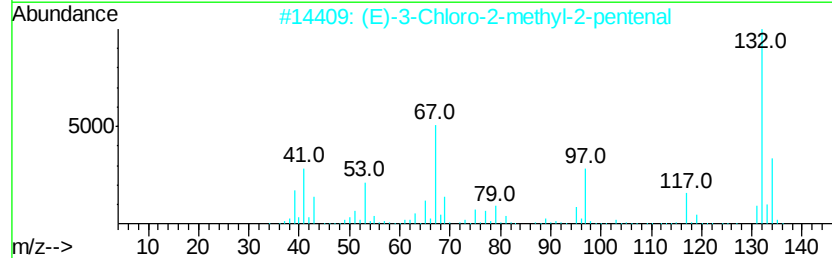
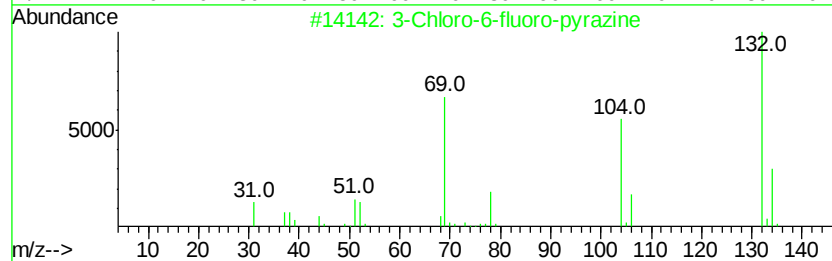
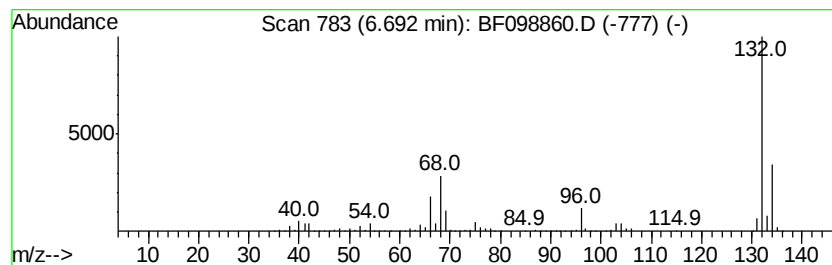
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	85.27 ng	3728970	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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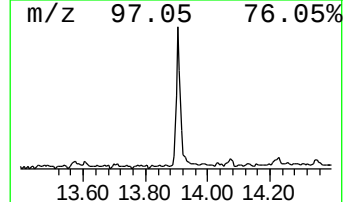
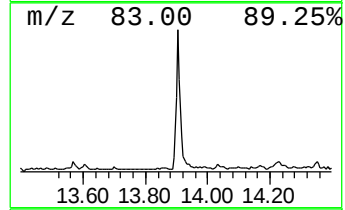
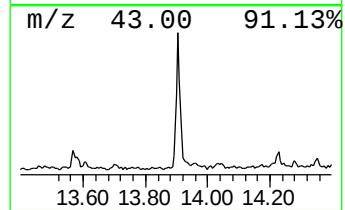
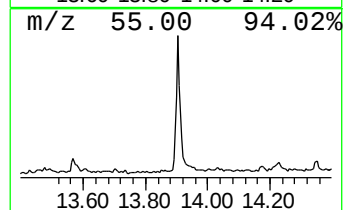
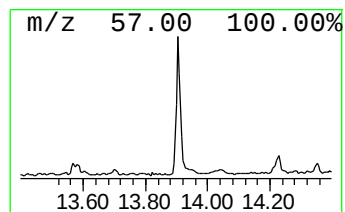
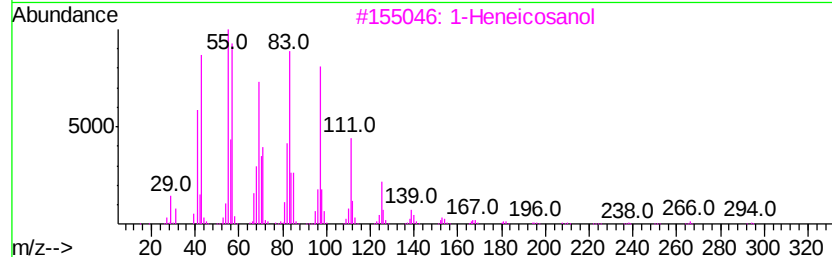
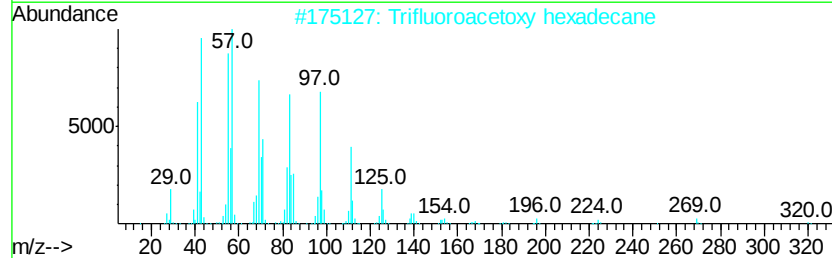
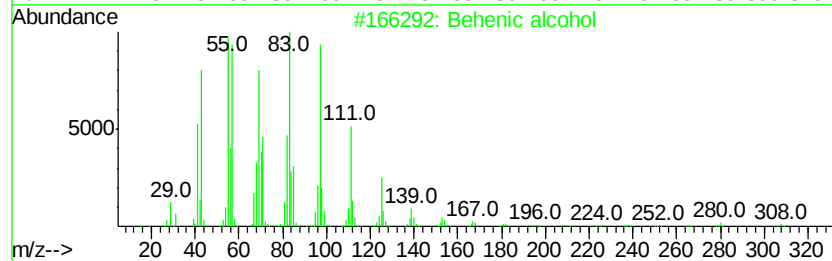
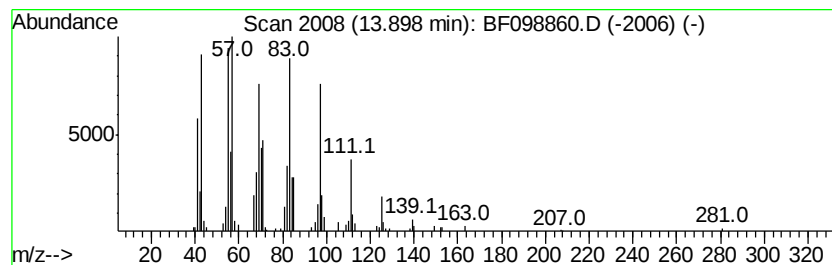
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	6.27 ng	264063	Chrysene-d12	14.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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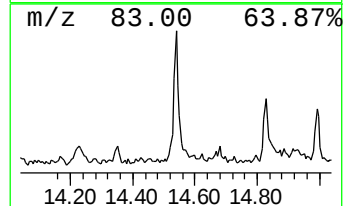
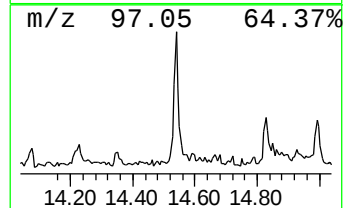
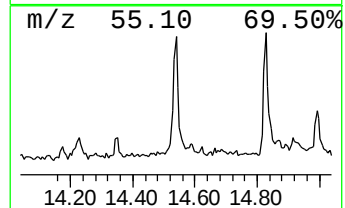
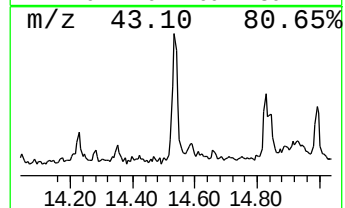
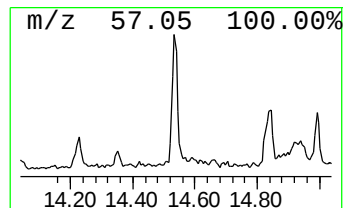
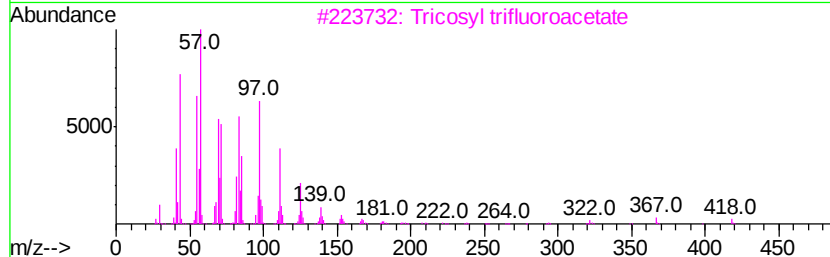
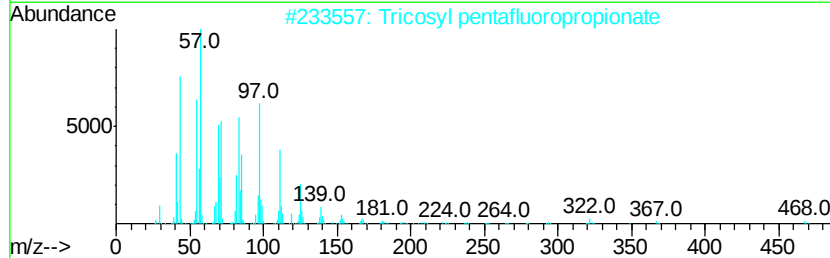
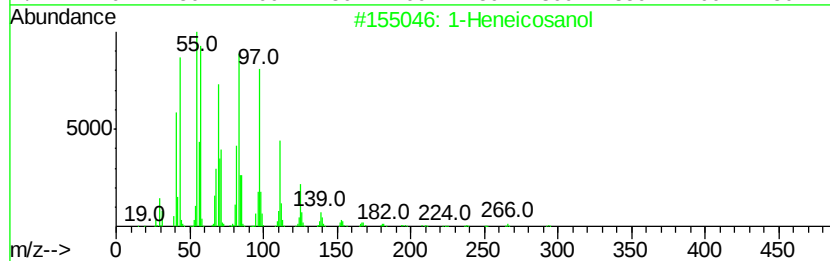
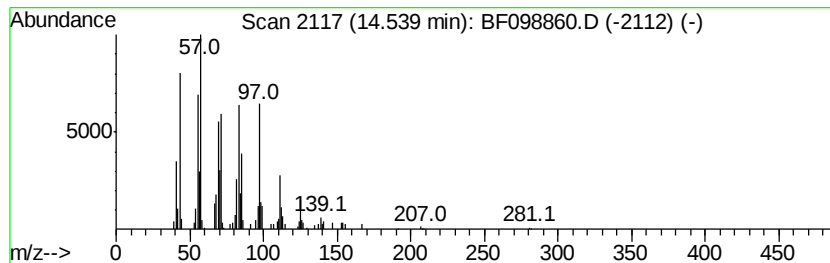
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.54	3.55 ng	149249	Chrysene-d12		14.07		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	92
2			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91
3			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
4			Eicosyl heptafluorobutyrte	494	C24H41F7O2	1000351-83-5	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098860.D
Acq On : 27 Sep 2017 13:50
Operator : SJ/JU
Sample : I5434-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

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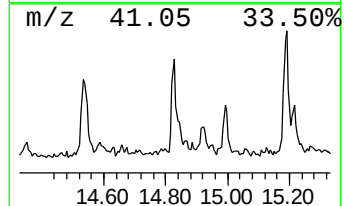
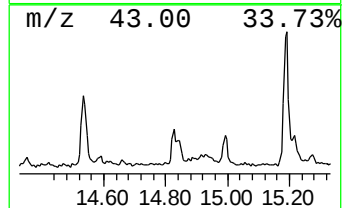
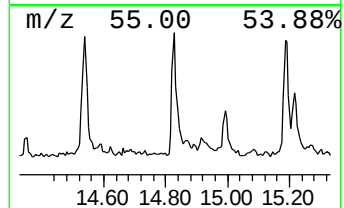
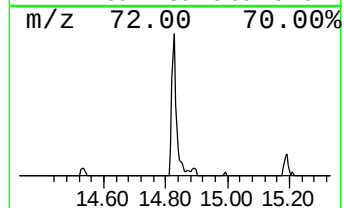
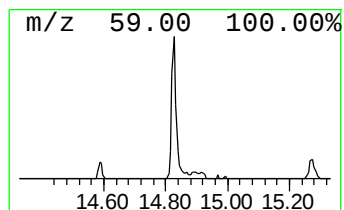
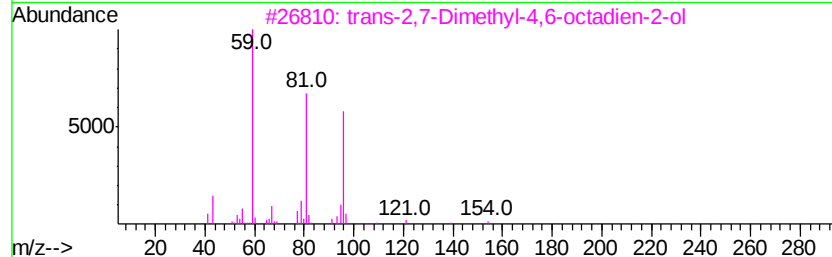
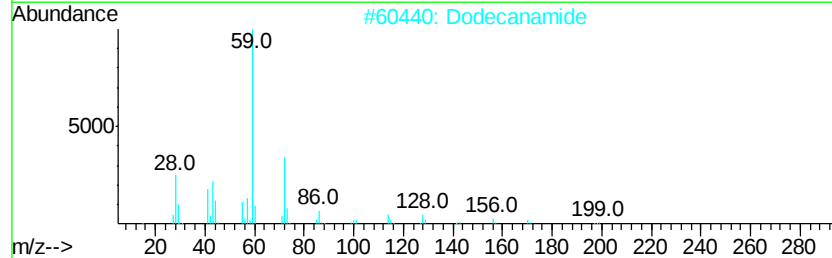
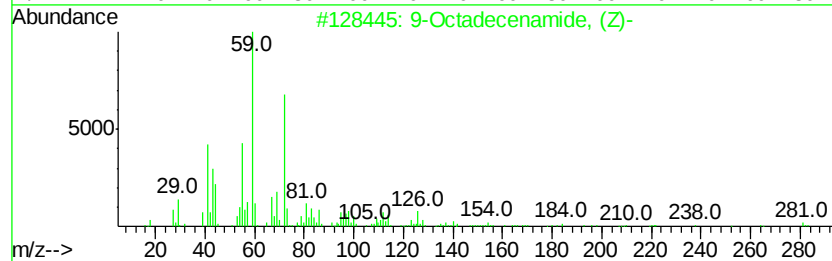
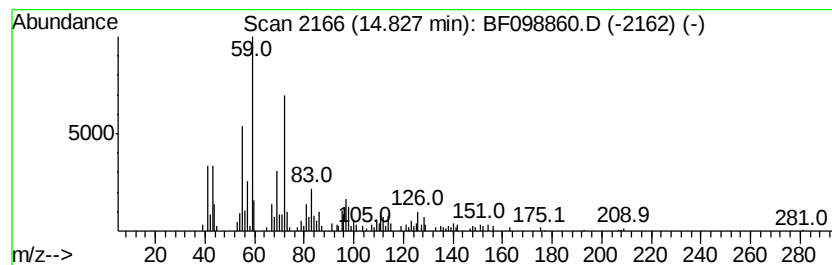
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.98 ng	152993	Perylene-d12	15.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2		Dodecanamide	199	C12H25NO	001120-16-7	47
3		trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1000281-69-5	38
4		Cyclohexanecarboxamide	127	C7H13NO	001122-56-1	38
5		Cyclopentylsilane	100	C5H12Si	080249-74-7	15



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098860.D
Acq On : 27 Sep 2017 13:50
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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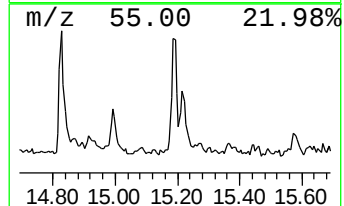
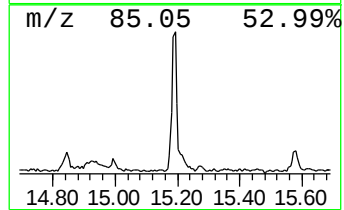
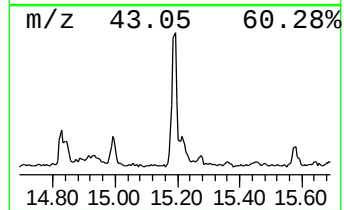
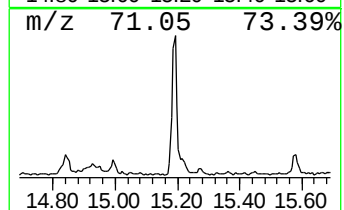
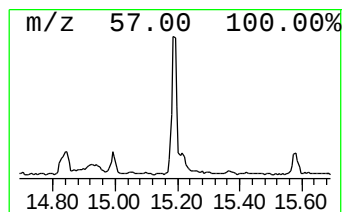
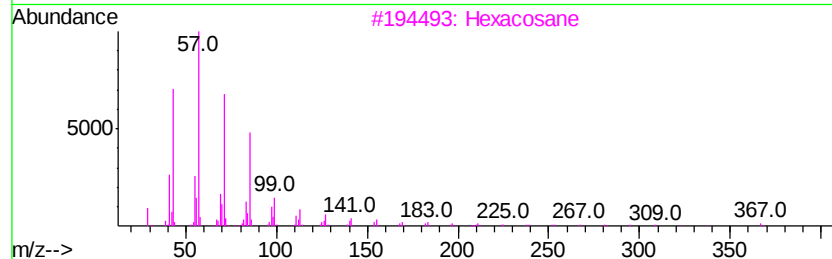
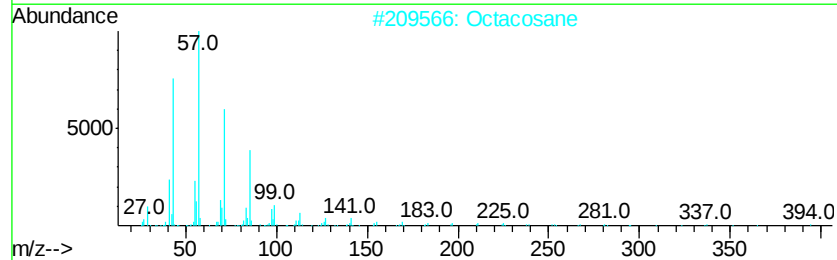
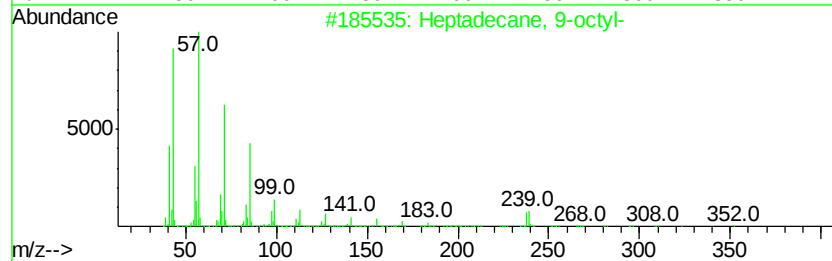
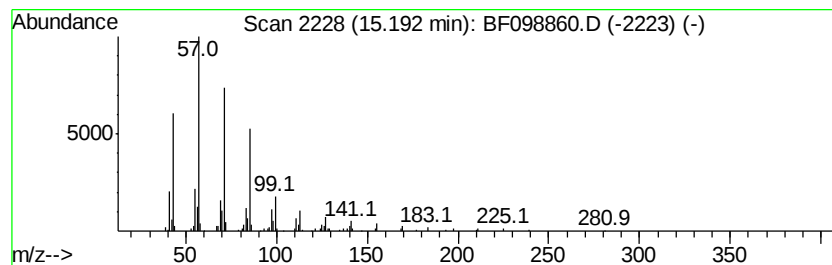
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	5.48 ng	210577	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
Data File : BF098860.D
Acq On : 27 Sep 2017 13:50
Operator : SJ/JU
Sample : I5434-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

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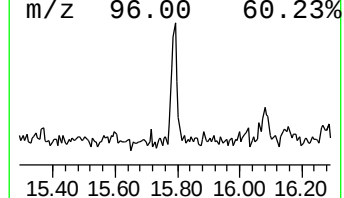
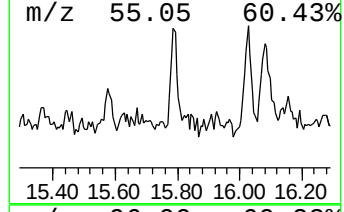
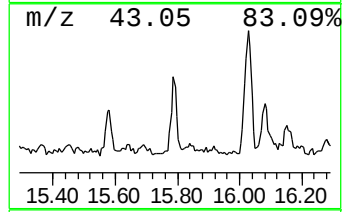
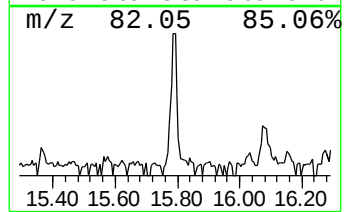
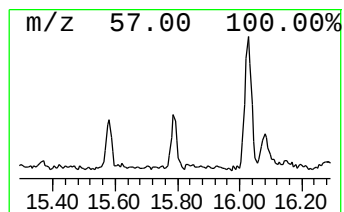
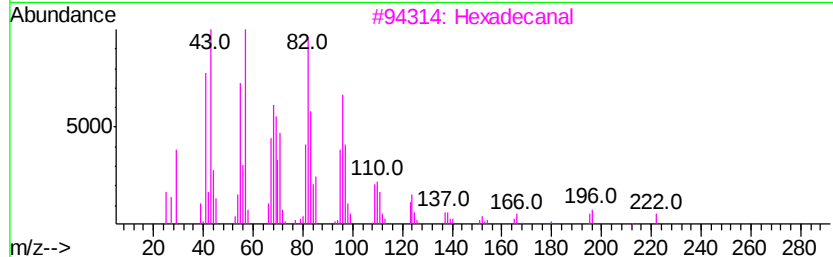
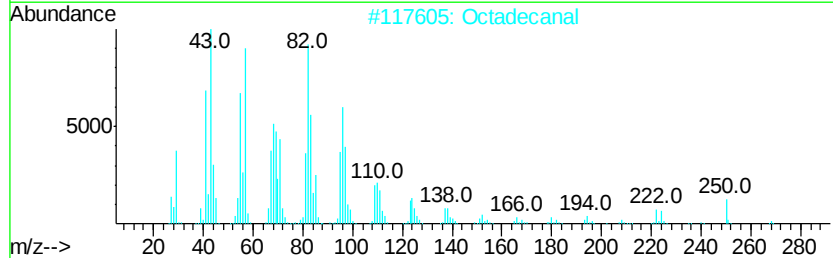
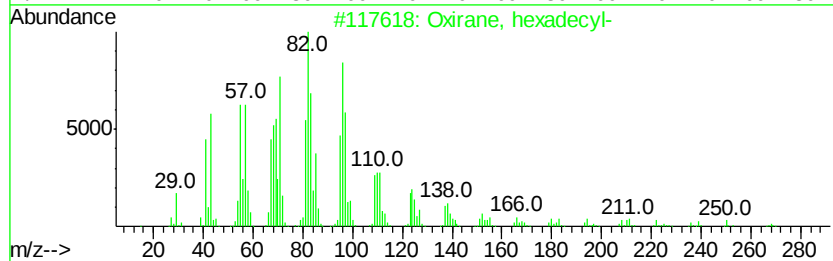
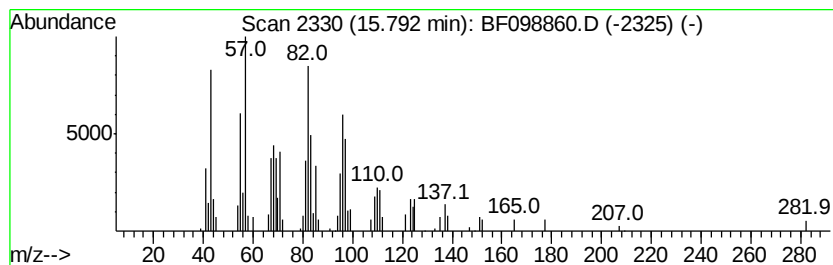
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Oxirane, hexadecyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	2.27 ng	87172	Perylene-d12	15.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2		Octadecanal	268	C18H36O	000638-66-4	91
3		Hexadecanal	240	C16H32O	000629-80-1	83
4		E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	70
5		1,19-Eicosadiene	278	C20H38	014811-95-1	58



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
Data File : BF098860.D
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Operator : SJ/JU
Sample : I5434-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

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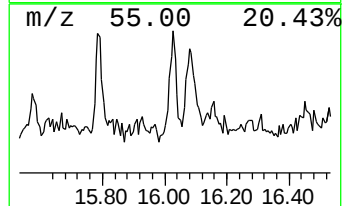
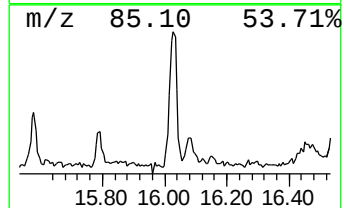
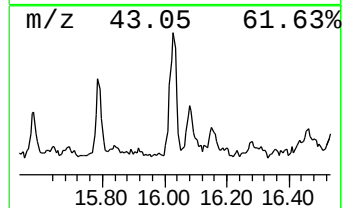
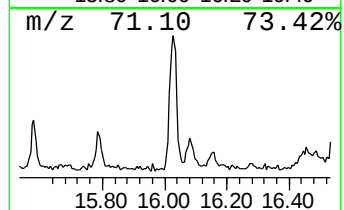
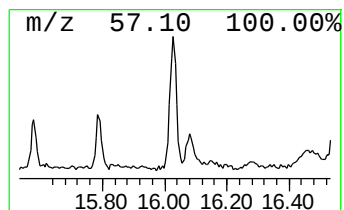
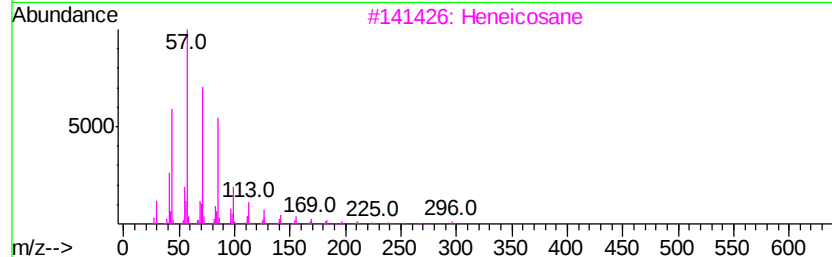
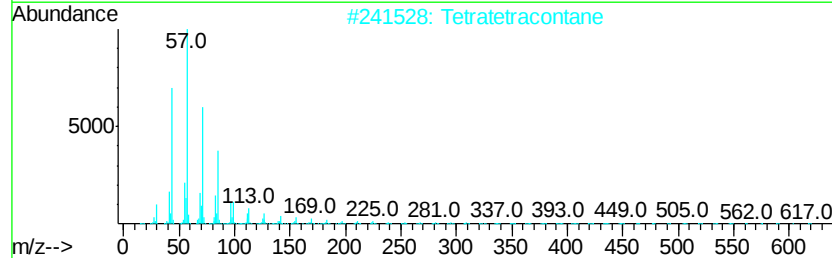
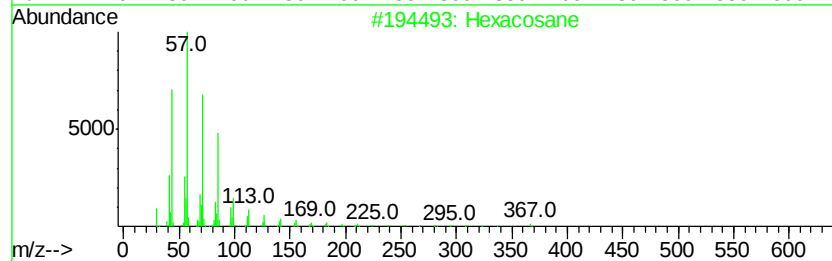
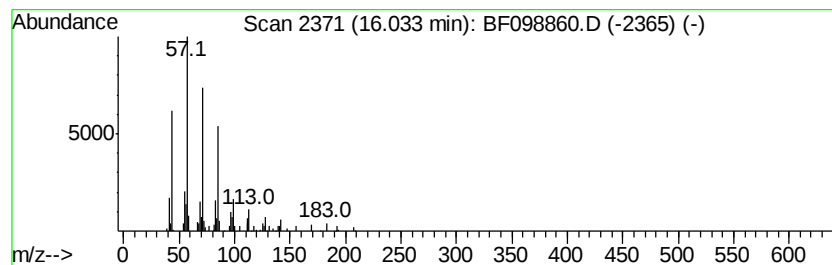
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	2.85 ng	109346	Perylene-d12	15.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Hentriacontane	437	C31H64	000630-04-6	91
5			triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
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Acq On : 27 Sep 2017 13:50
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Misc :
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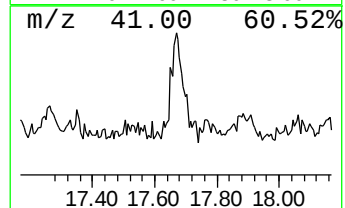
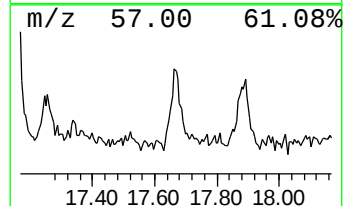
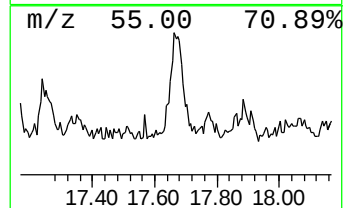
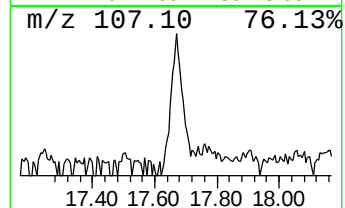
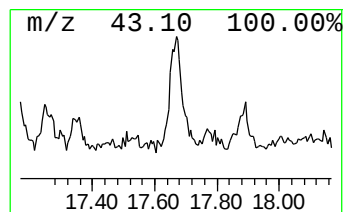
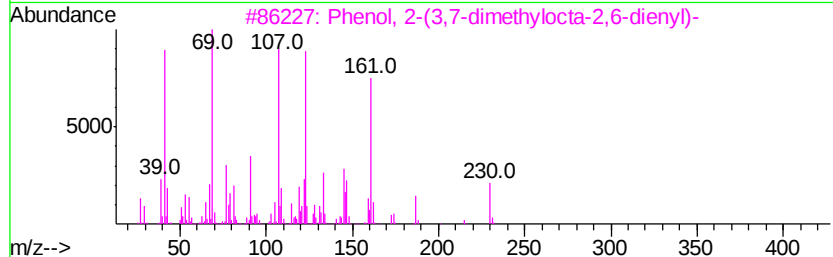
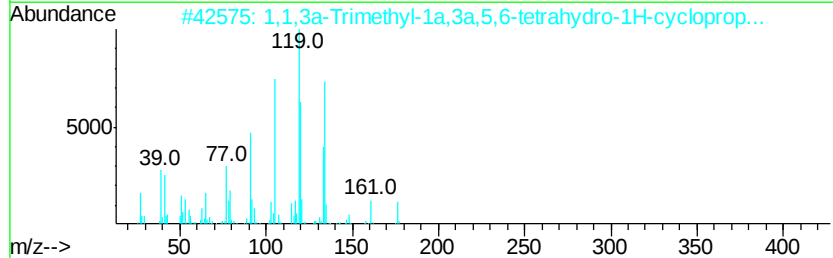
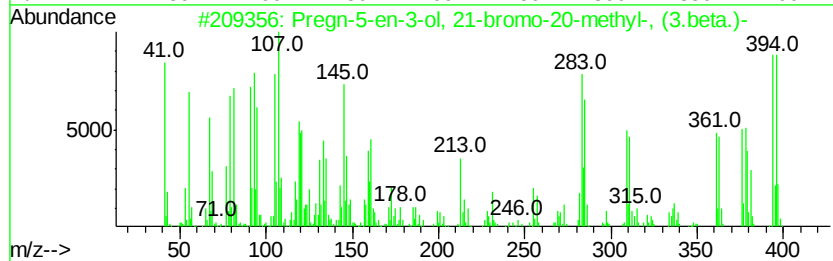
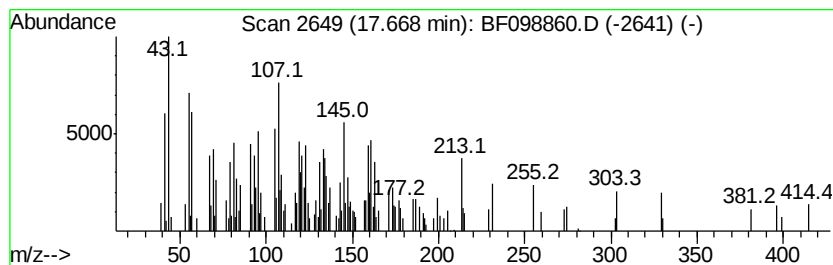
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown17.67 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.67	8.09 ng	310637	Perylene-d12	15.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	18
2		1,1,3a-Trimethyl-1a,3a,5,6-tetra...	176	C12H16O	091531-54-3	18
3		Phenol, 2-(3,7-dimethylocta-2,6-...	230	C16H22O	010232-02-7	14
4		1H-Cyclopropylazulen-4-ol, deca...	222	C15H26O	000552-02-3	14
5		cis-p-Mentha-2,8-dien-1-ol	152	C10H16O	003886-78-0	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF092717\
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Sample : I5434-12
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.15	18.1	ng	793128	1	6.92	874599	20.0
unknown6.69	6.69	85.3	ng	3728970	1	6.92	874599	20.0
Behenic alcohol	13.90	6.3	ng	264063	5	14.07	841702	20.0
1-Heneicosanol	14.54	3.5	ng	149249	5	14.07	841702	20.0
9-Octadecenamide, ...	14.83	4.0	ng	152993	6	15.56	768308	20.0
Heptadecane, 9-oc...	15.19	5.5	ng	210577	6	15.56	768308	20.0
Oxirane, hexadecyl-	15.79	2.3	ng	87172	6	15.56	768308	20.0
Hexacosane	16.03	2.9	ng	109346	6	15.56	768308	20.0
unknown17.67	17.67	8.1	ng	310637	6	15.56	768308	20.0
Naphthalene, 1,2,...	18.51	2.7	ng	102228	6	15.56	768308	20.0