

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
 Data File : BF095723.D
 Acq On : 6 Jun 2017 22:40
 Operator : SJ/MA
 Sample : I3478-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 337-COMP

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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	1.810	35	38	48	rVB4	14649	30024	1.34%	0.161%
2	4.604	509	513	532	rBV	57049	175737	7.87%	0.942%
3	5.275	623	627	659	rBV	1153235	1943154	86.98%	10.415%
4	6.939	905	910	922	rBV	1240711	1871549	83.78%	10.031%
5	7.039	922	927	937	rVB	1530876	2125061	95.12%	11.390%
6	7.381	981	985	1001	rBB	378461	488787	21.88%	2.620%
7	7.622	1020	1026	1044	rBV	1169677	1606515	71.91%	8.610%
8	8.298	1136	1141	1175	rBV	856574	1198877	53.66%	6.426%
9	9.410	1326	1330	1346	rBV	485311	647256	28.97%	3.469%
10	11.198	1627	1634	1650	rBV	1691019	2234009	100.00%	11.974%
11	11.886	1747	1751	1764	rBV	167069	203256	9.10%	1.089%
12	12.233	1805	1810	1816	rBV2	547897	660187	29.55%	3.538%
13	12.280	1816	1818	1826	rVB3	18303	22880	1.02%	0.123%
14	13.098	1950	1957	1962	rBV	25721	32654	1.46%	0.175%
15	13.527	2025	2030	2044	rVV	817963	1070276	47.91%	5.736%
16	13.863	2083	2087	2094	rBV	27612	41392	1.85%	0.222%
17	14.627	2213	2217	2222	rVV	462142	594117	26.59%	3.184%
18	14.663	2222	2223	2233	rVB	33711	46346	2.07%	0.248%
19	15.157	2302	2307	2313	rBV2	16477	23062	1.03%	0.124%
20	15.645	2385	2390	2396	rBV2	132451	161520	7.23%	0.866%
21	16.445	2519	2526	2532	rBV	71732	86697	3.88%	0.465%
22	16.751	2572	2578	2586	rBV	106852	149231	6.68%	0.800%
23	16.998	2615	2620	2624	rBV	1304214	1535222	68.72%	8.228%
24	18.256	2829	2834	2843	rBV2	97275	152794	6.84%	0.819%
25	18.339	2843	2848	2853	rBV	413841	472546	21.15%	2.533%
26	18.421	2858	2862	2866	rVB	24998	30387	1.36%	0.163%
27	19.056	2966	2970	2978	rVB	28660	40160	1.80%	0.215%
28	19.492	3040	3044	3047	rVB	40293	42831	1.92%	0.230%
29	19.574	3054	3058	3062	rBV2	59401	63957	2.86%	0.343%
30	19.615	3062	3065	3069	rBV	30683	38520	1.72%	0.206%
31	19.797	3089	3096	3103	rBV2	84794	168287	7.53%	0.902%
32	19.962	3121	3124	3128	rVB	27870	27592	1.24%	0.148%
33	20.003	3128	3131	3144	rBV	321561	417748	18.70%	2.239%
34	20.274	3174	3177	3184	rVB7	17653	27181	1.22%	0.146%

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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	20.462	3204	3209	3212	rBV	51983	73414	3.29%	0.393%
36	20.492	3212	3214	3220	rVB6	25601	38777	1.74%	0.208%
37	21.039	3303	3307	3314	rBV5	18588	31231	1.40%	0.167%
38	21.268	3342	3346	3351	rVB3	17244	31281	1.40%	0.168%
39	21.550	3389	3394	3398	rBV5	10638	25495	1.14%	0.137%
40	23.033	3641	3646	3654	rVB9	11596	27725	1.24%	0.149%

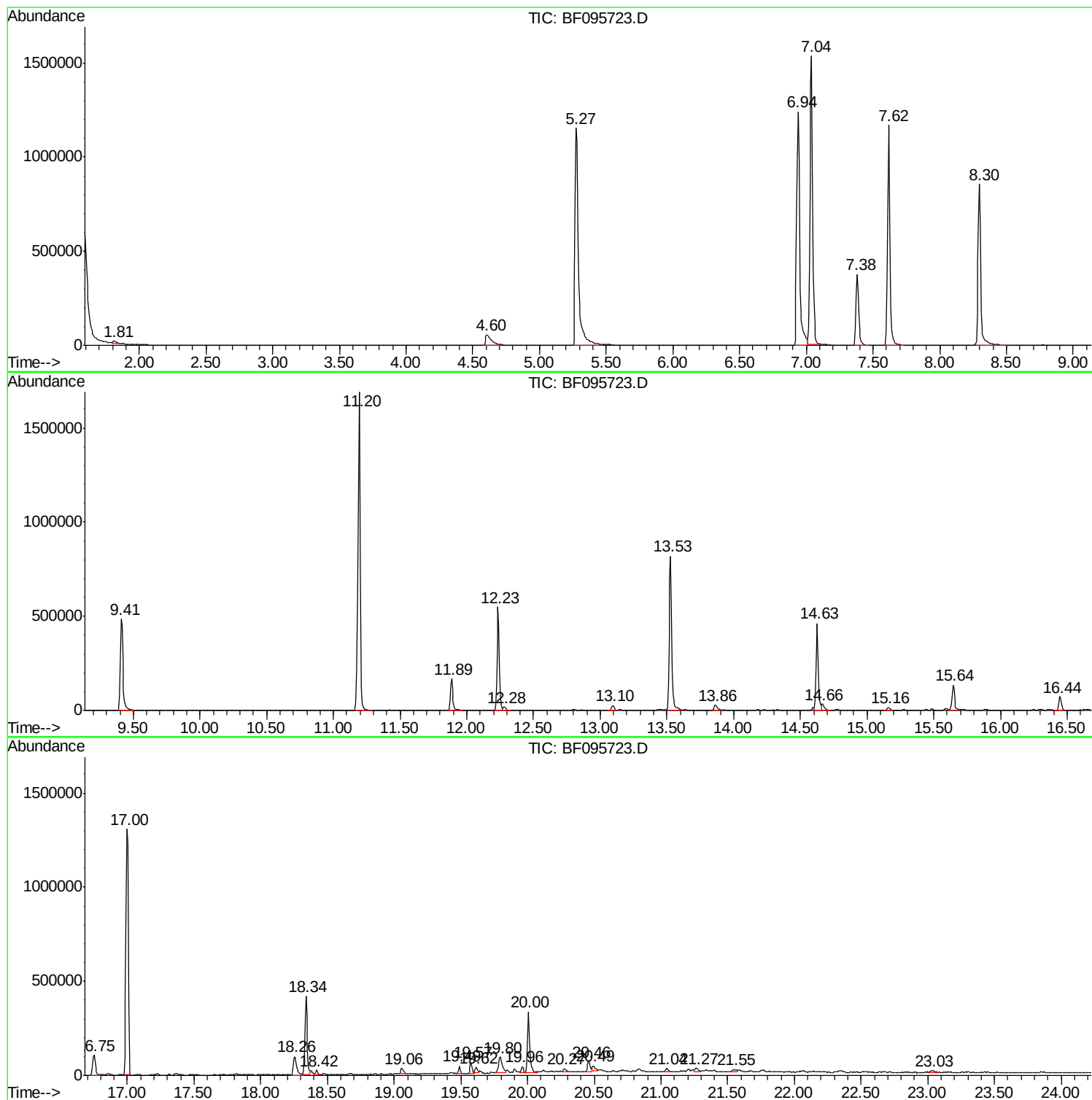
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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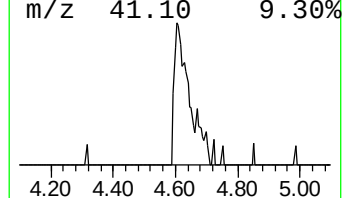
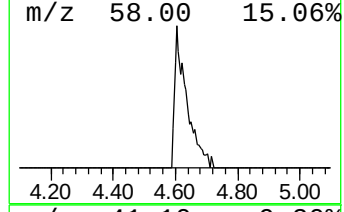
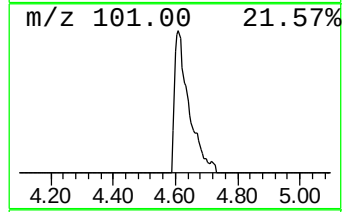
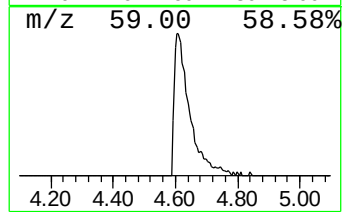
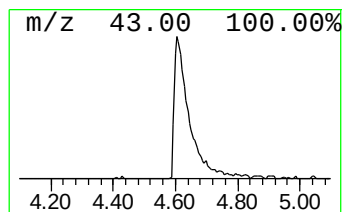
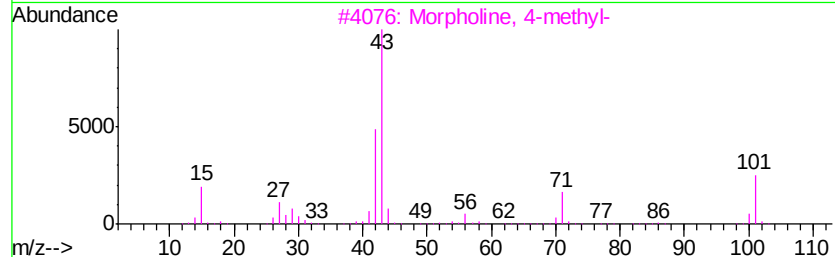
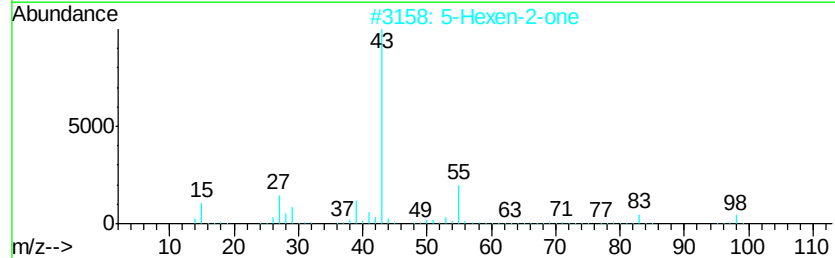
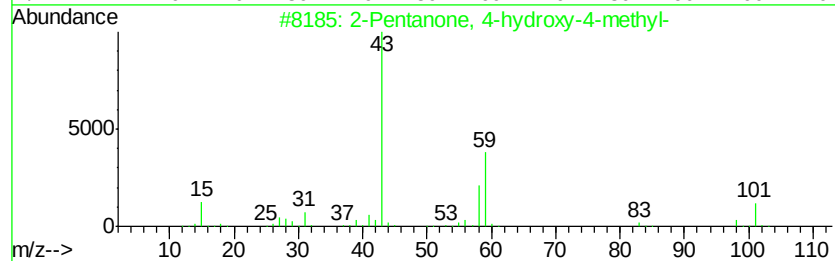
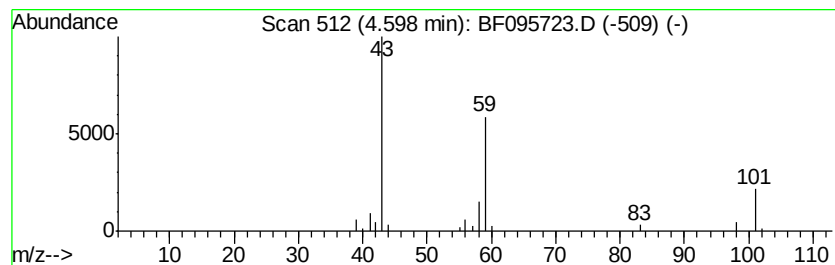
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.60	7.19 ng	175737	1,4-Dichlorobenzene-d4	7.38

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2			5-Hexen-2-one	98	C6H10O	000109-49-9	9
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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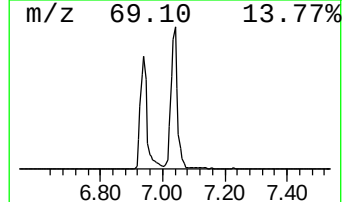
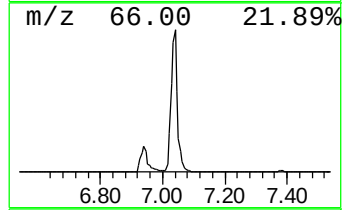
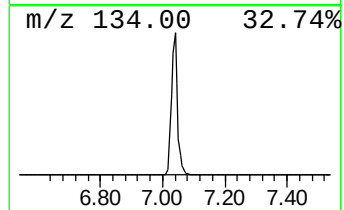
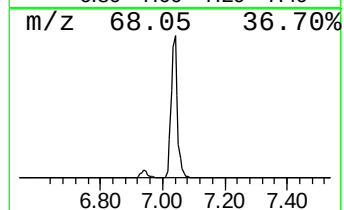
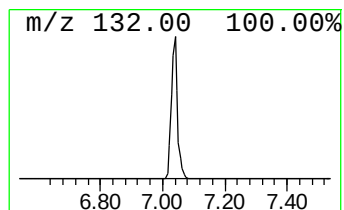
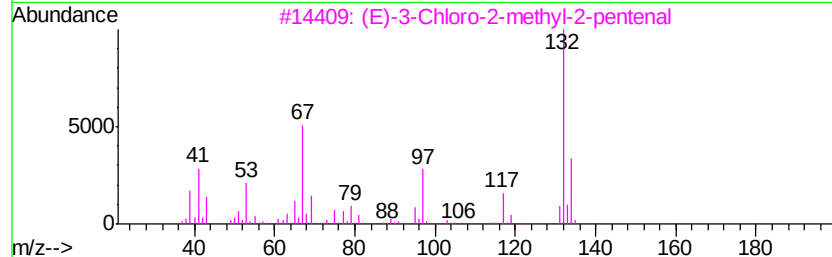
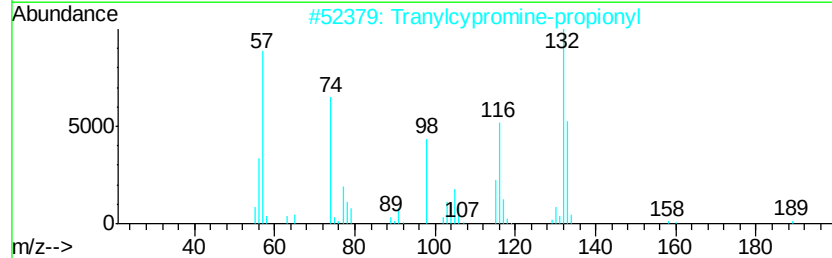
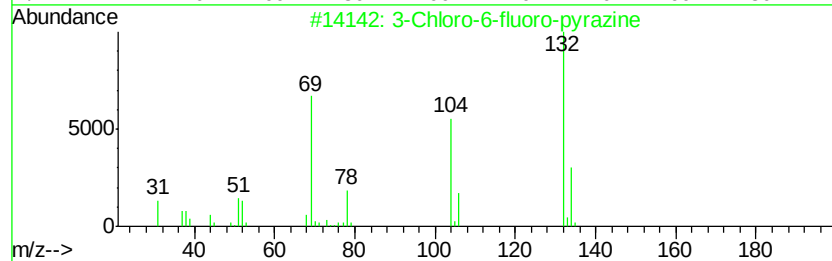
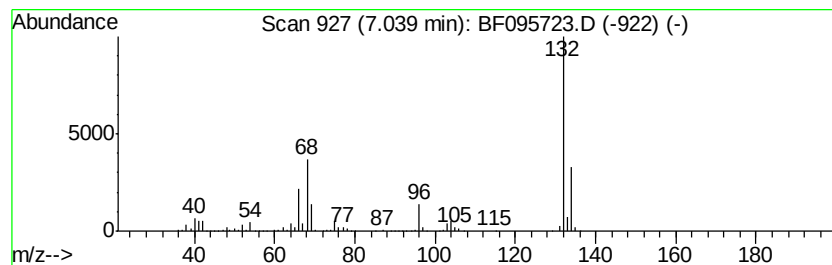
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	86.95 ng	2125060	1,4-Dichlorobenzene-d4	7.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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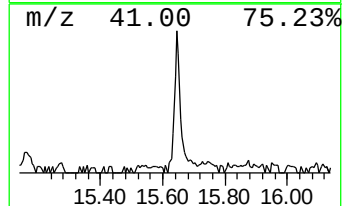
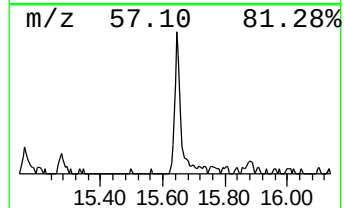
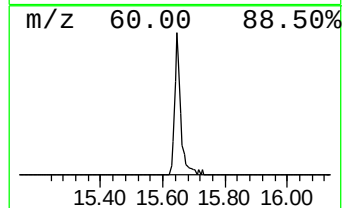
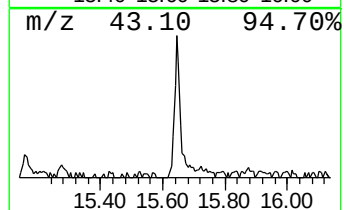
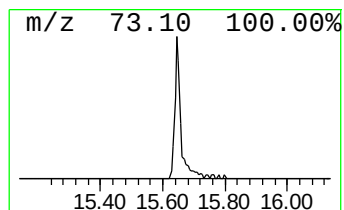
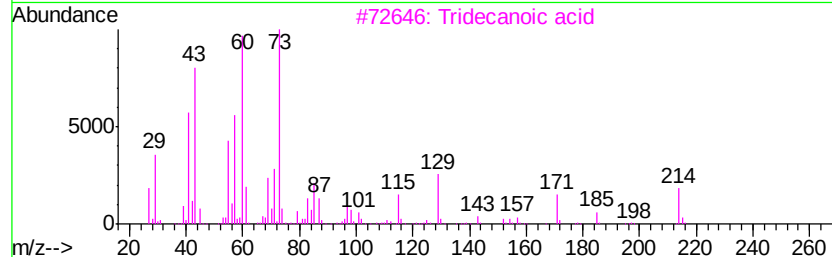
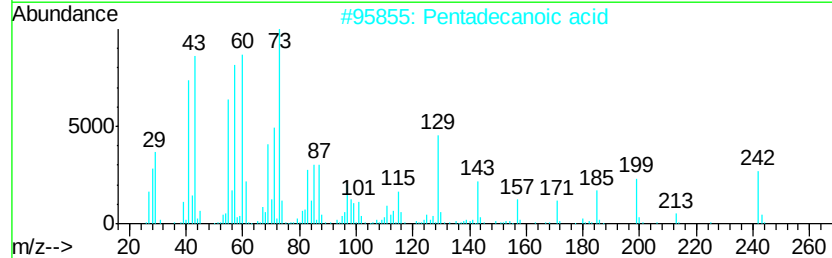
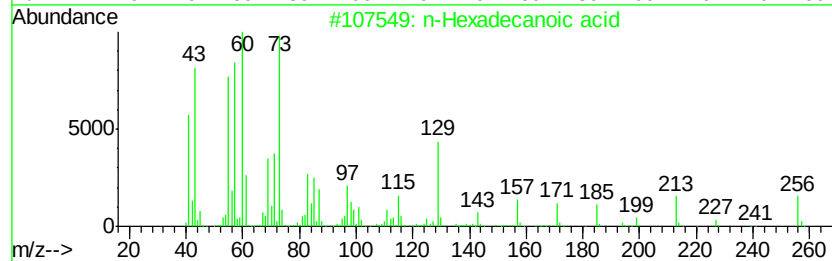
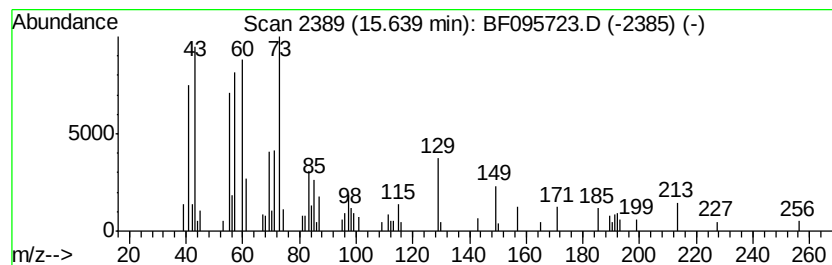
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	5.44 ng	161520	Phenanthrene-d10	14.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		Dodecanoic acid	200	C12H24O2	000143-07-7	52



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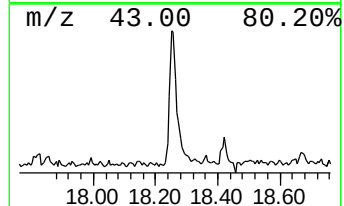
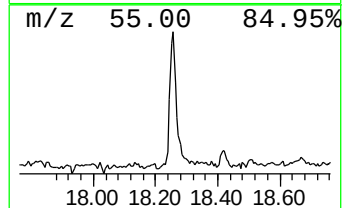
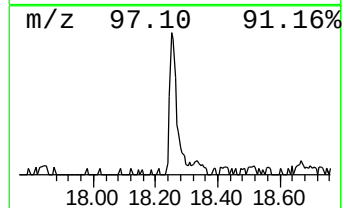
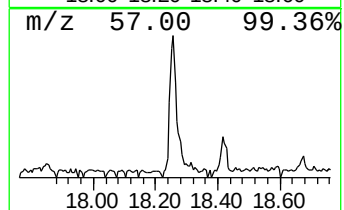
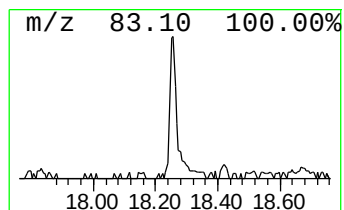
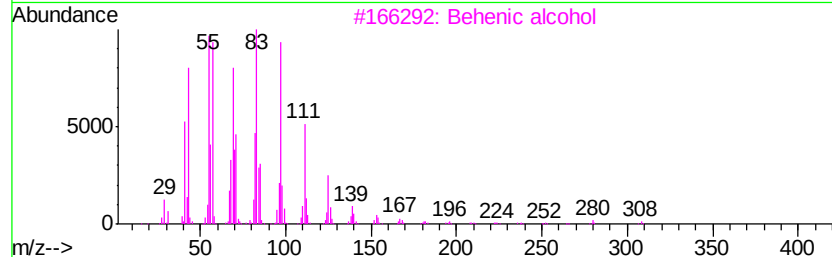
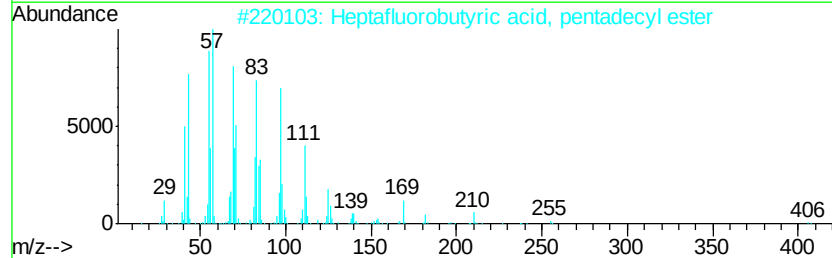
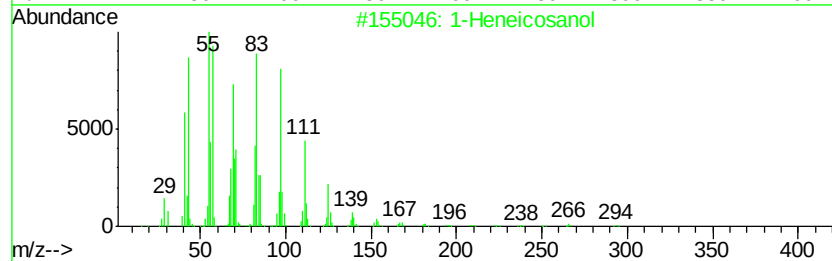
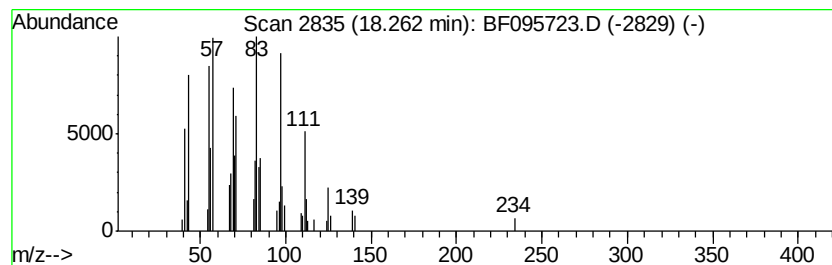
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.26	6.47 ng	152794	Chrysene-d12		18.34	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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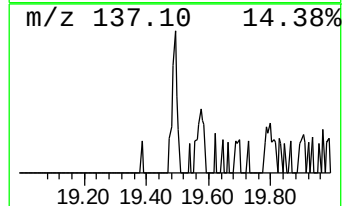
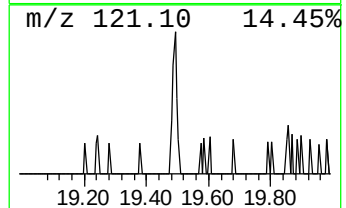
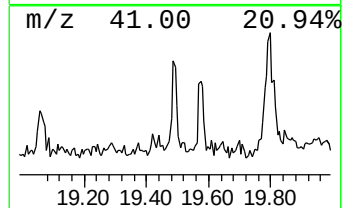
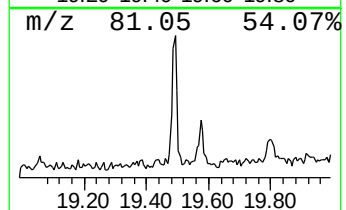
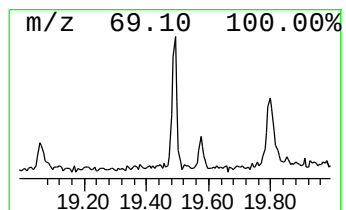
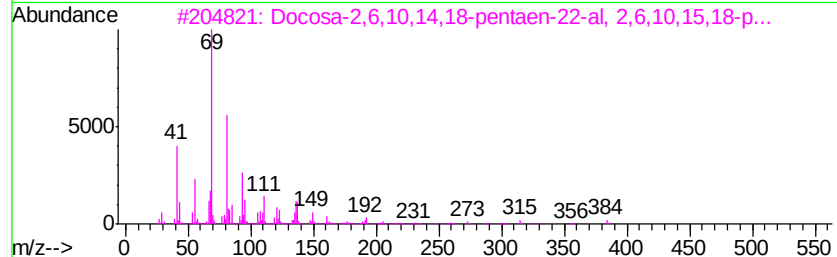
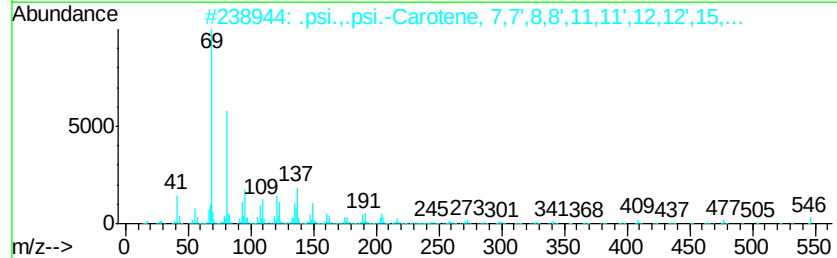
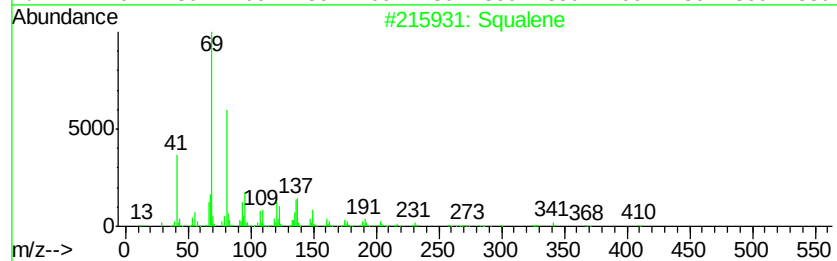
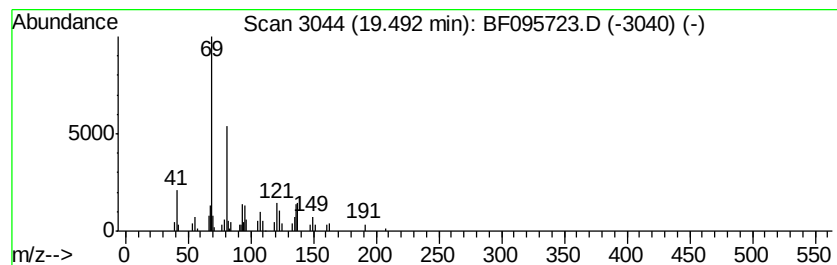
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.49	2.05 ng	42831	Perylene-d12	20.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	000111-02-4 91
2	.psi.,.psi.-Carotene, 7,7',8,8',...		547 C40H66	000502-62-5 90
3	Docosa-2,6,10,14,18-pentaen-22-a...		384 C27H44O	1000163-04-7 90
4	Supraene		410 C30H50	007683-64-9 80
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...		222 C15H26O	004602-84-0 72



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Data File : BF095723.D
Acq On : 6 Jun 2017 22:40
Operator : SJ/MA
Sample : I3478-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

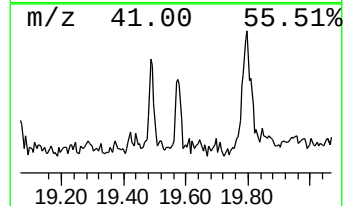
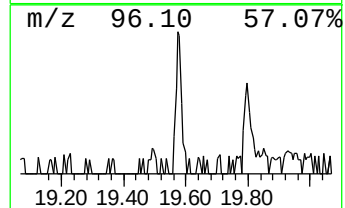
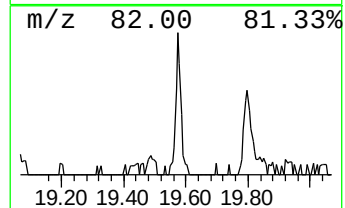
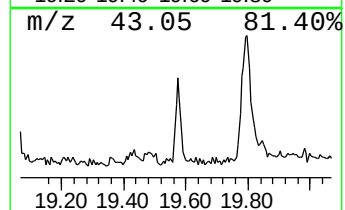
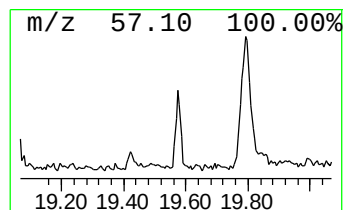
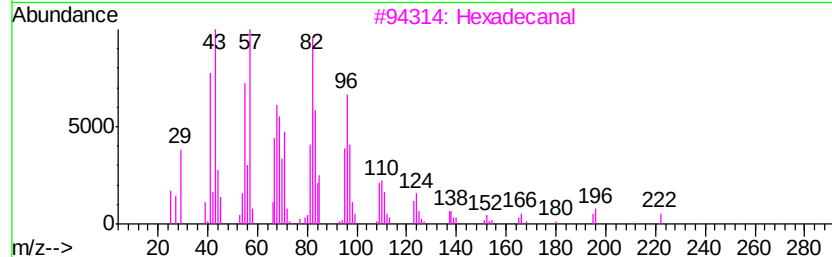
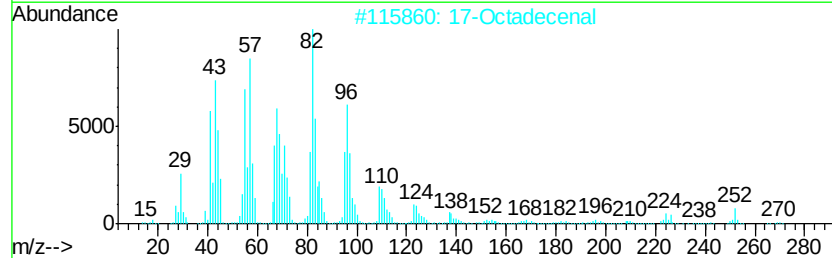
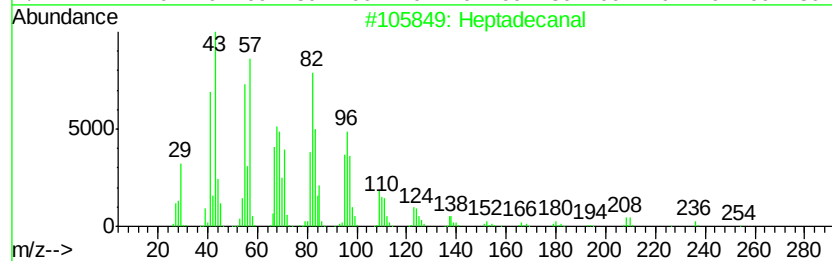
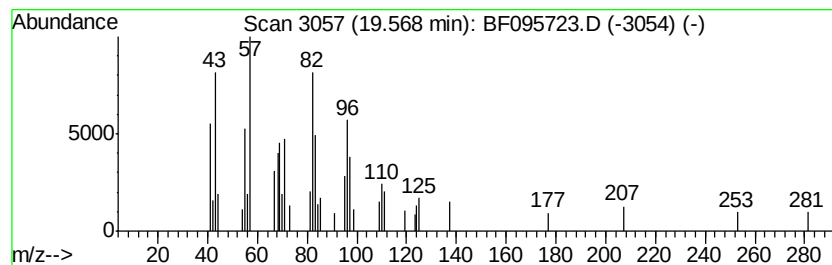
Instrument :
BNA_F
ClientSampleId :
337-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.57	3.06 ng	63957	Perylene-d12		20.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanal	254	C17H34O	1000376-70-0	90
2	17-Octadecenal	266	C18H34O	056554-86-0	87
3	Hexadecanal	240	C16H32O	000629-80-1	83
4	16-Octadecenal	266	C18H34O	056554-87-1	80
5	14-Heptadecenal	252	C17H32O	1000144-58-0	80



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
Data File : BF095723.D
Acq On : 6 Jun 2017 22:40
Operator : SJ/MA
Sample : I3478-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

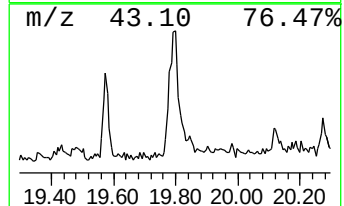
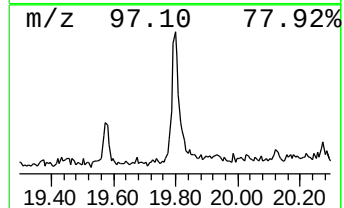
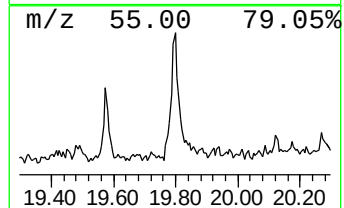
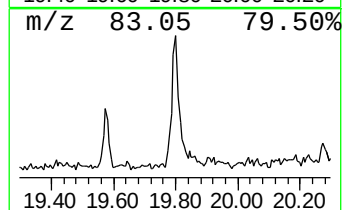
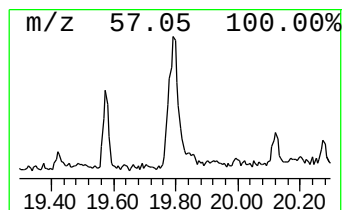
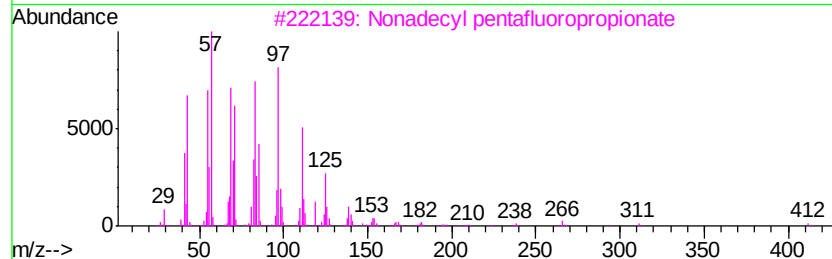
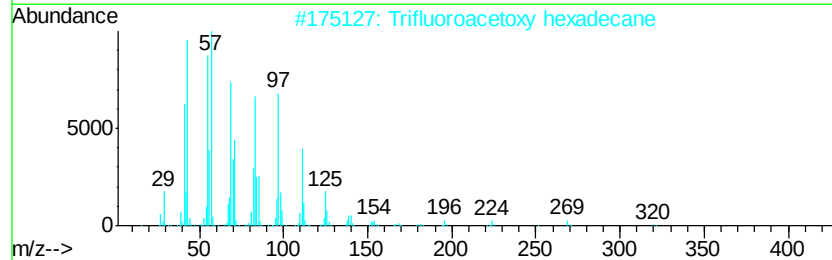
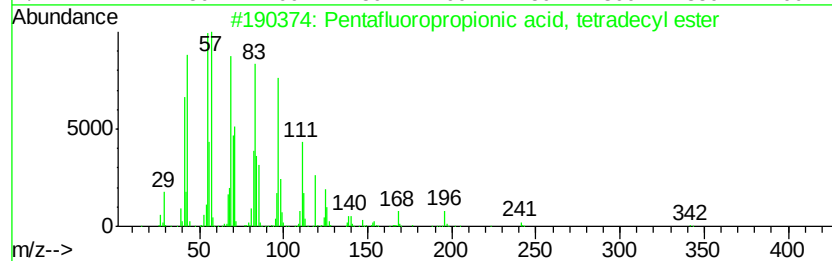
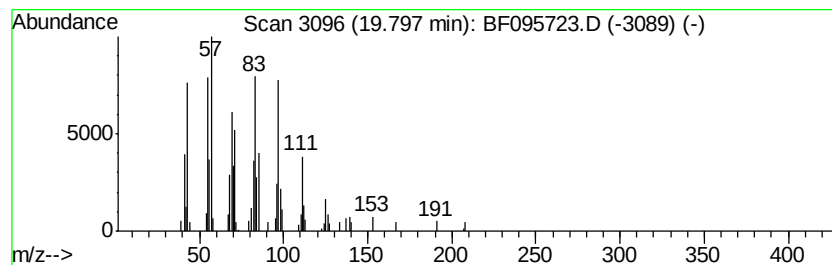
Instrument :
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ClientSampleId :
337-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
19.80	8.06 ng	168287	Perylene-d12	20.01		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90
3		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
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Acq On : 6 Jun 2017 22:40
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Sample : I3478-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

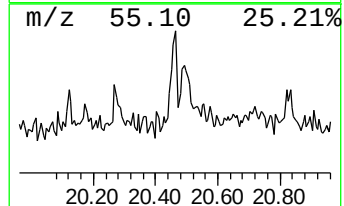
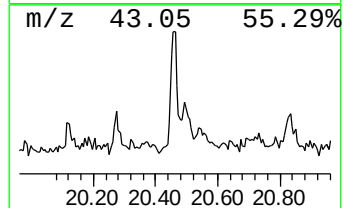
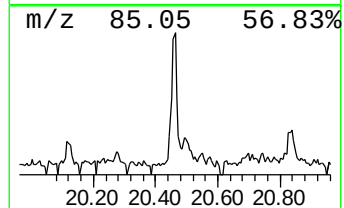
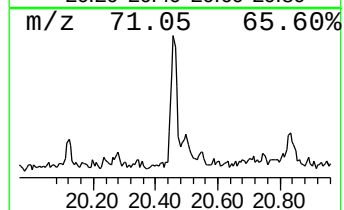
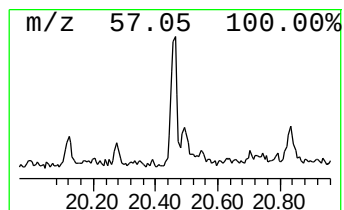
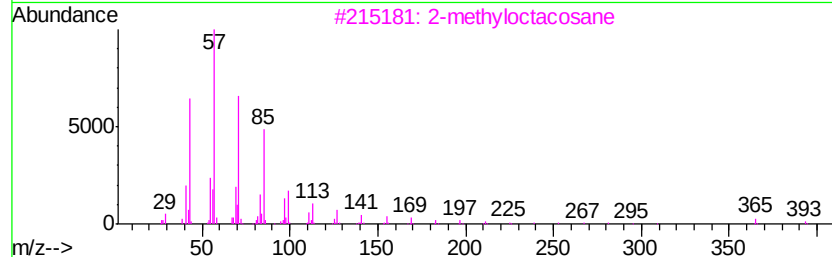
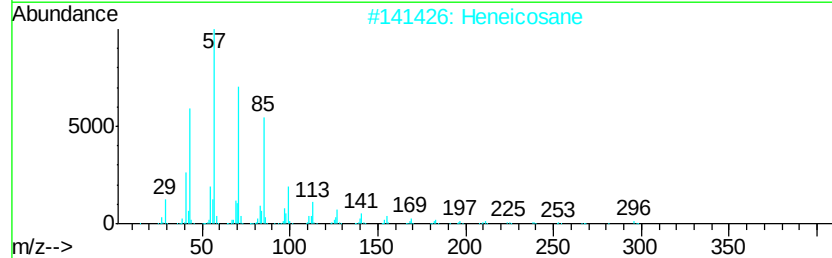
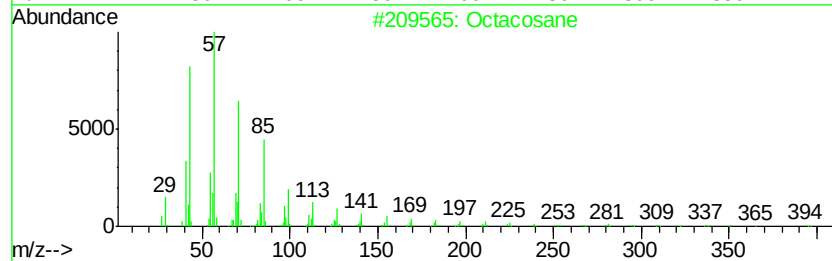
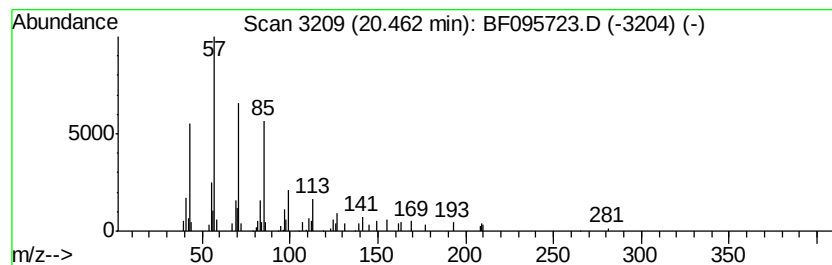
Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
20.46	3.51 ng	73414	Perylene-d12		20.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	86
4	Triacontane	422	C30H62	000638-68-6	86
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060617\
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Operator : SJ/MA
Sample : I3478-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
337-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.60	7.2	ng	175737	1	7.38	488787	20.0
unknown7.04	7.04	87.0	ng	2125060	1	7.38	488787	20.0
n-Hexadecanoic acid	15.64	5.4	ng	161520	4	14.63	594117	20.0
1-Heneicosanol	18.26	6.5	ng	152794	5	18.34	472546	20.0
Squalene	19.49	2.0	ng	42831	6	20.01	417748	20.0
Heptadecanal	19.57	3.1	ng	63957	6	20.01	417748	20.0
Pentafluoropropio...	19.80	8.1	ng	168287	6	20.01	417748	20.0
Octacosane	20.46	3.5	ng	73414	6	20.01	417748	20.0