

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
 Data File : BM017253.D
 Acq On : 20 Oct 2018 06:37
 Operator : MJ/SJ
 Sample : J5575-14
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SSSI-1015-S-DH-25-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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.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	4.834	309	314	321	rBV	190890	271246	1.91%	0.281%
2	5.281	383	390	401	rBV	4759296	6767869	47.61%	7.003%
3	6.846	646	656	669	rBV	4791060	7896040	55.54%	8.170%
4	7.198	707	716	728	rBV	4860439	7554956	53.14%	7.817%
5	7.663	788	795	803	rBV	1131534	1743414	12.26%	1.804%
6	7.981	841	849	858	rVB	3581290	5692951	40.04%	5.890%
7	8.816	983	991	1000	rBV	2947564	4679158	32.91%	4.841%
8	10.439	1260	1267	1280	rBV	1477003	2449723	17.23%	2.535%
9	12.922	1681	1689	1699	rBV	7569919	11165640	78.54%	11.553%
10	13.769	1828	1833	1844	rVB	676525	984347	6.92%	1.018%
11	14.304	1917	1924	1932	rBV2	2248832	3332943	23.44%	3.448%
12	15.798	2172	2178	2201	rBV	5695867	8460678	59.51%	8.754%
13	17.057	2385	2392	2397	rBV	2617182	3890493	27.37%	4.025%
14	17.962	2536	2546	2555	rBV	434986	664471	4.67%	0.688%
15	19.121	2736	2743	2752	rBV	142515	257985	1.81%	0.267%
16	19.245	2760	2764	2773	rBV3	148479	218135	1.53%	0.226%
17	19.398	2786	2790	2796	rBV2	235104	306631	2.16%	0.317%
18	19.480	2800	2804	2808	rVB2	128268	162601	1.14%	0.168%
19	19.692	2834	2840	2846	rBV	10786866	14216611	100.00%	14.709%
20	20.392	2954	2959	2965	rBV	627724	1222145	8.60%	1.265%
21	20.445	2965	2968	2975	rVV2	500717	708750	4.99%	0.733%
22	20.509	2975	2979	2983	rVV2	245124	344936	2.43%	0.357%
23	20.974	3054	3058	3070	rBV	631652	1062681	7.47%	1.100%
24	21.251	3099	3105	3117	rBV	3408020	4419165	31.08%	4.572%
25	21.356	3120	3123	3128	rBV4	110777	192424	1.35%	0.199%
26	21.409	3129	3132	3137	rVB	350694	412032	2.90%	0.426%
27	21.845	3202	3206	3209	rBV	406722	504556	3.55%	0.522%
28	22.098	3245	3249	3254	rBV	400955	499040	3.51%	0.516%
29	22.297	3280	3283	3289	rVB	459515	607475	4.27%	0.629%
30	22.427	3302	3305	3310	rVB	235071	302986	2.13%	0.313%
31	22.797	3364	3368	3375	rVB	492258	668845	4.70%	0.692%
32	23.356	3459	3463	3470	rVB	414028	672018	4.73%	0.695%
33	23.462	3474	3481	3491	rVB	2006829	3824302	26.90%	3.957%
34	23.992	3567	3571	3578	rVB2	284311	492057	3.46%	0.509%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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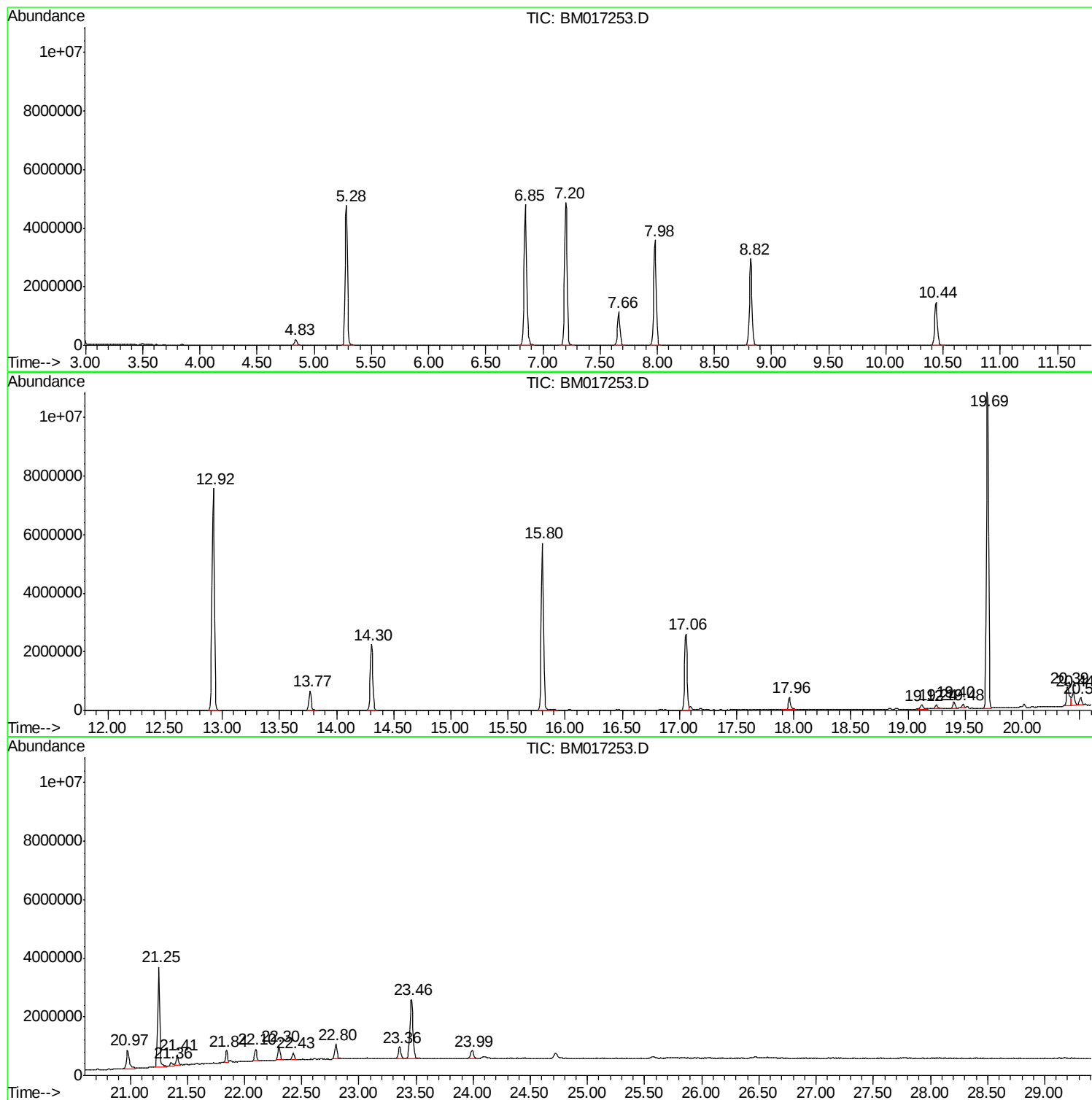
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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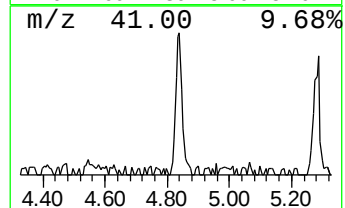
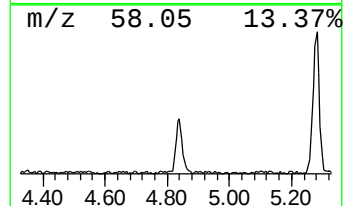
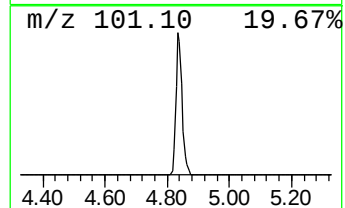
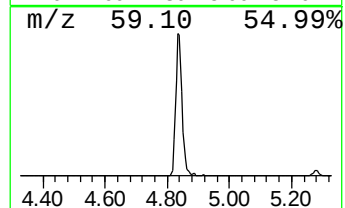
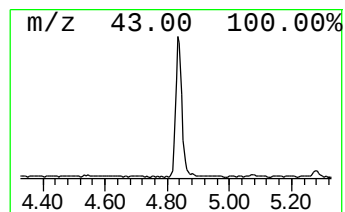
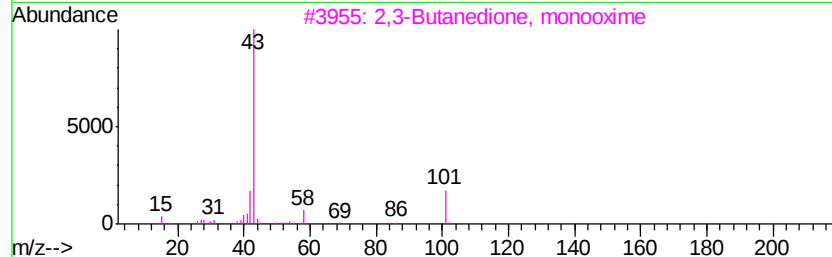
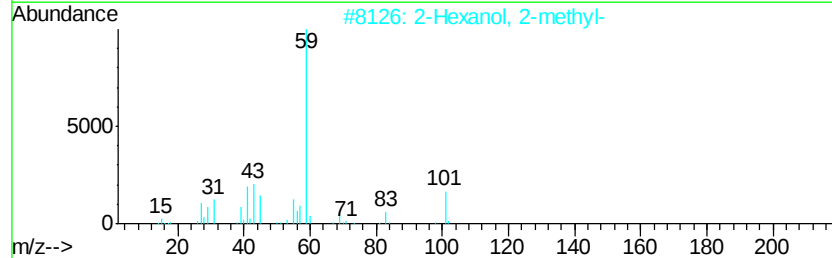
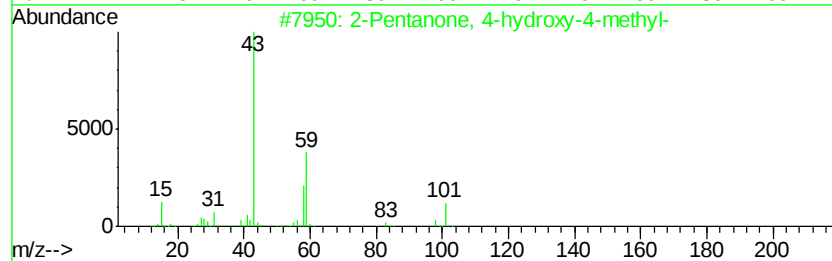
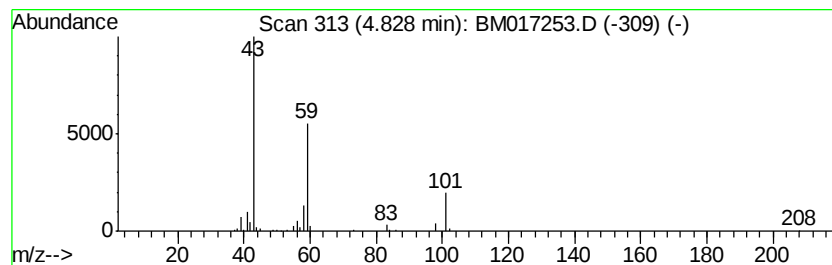
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	3.11 ng	271246	1,4-Dichlorobenzene-d4	7.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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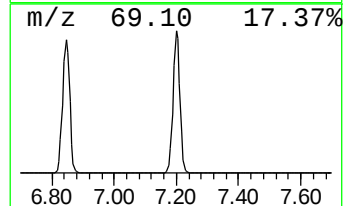
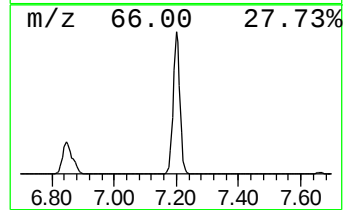
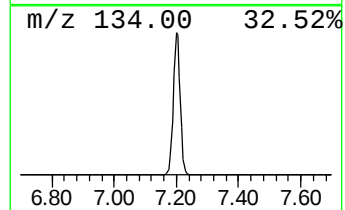
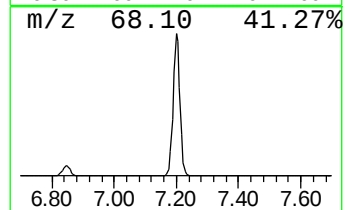
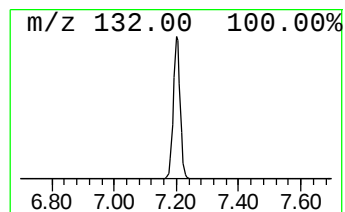
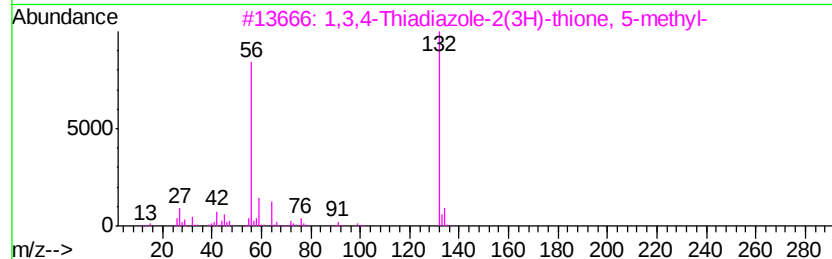
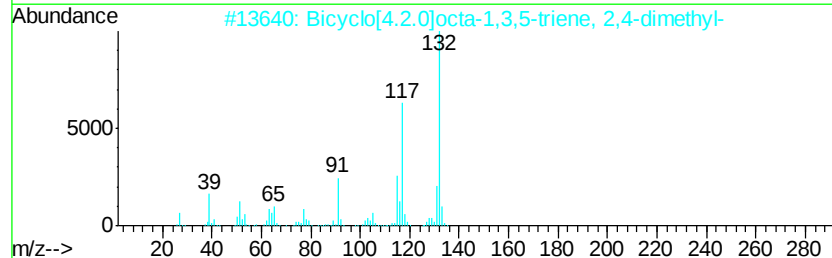
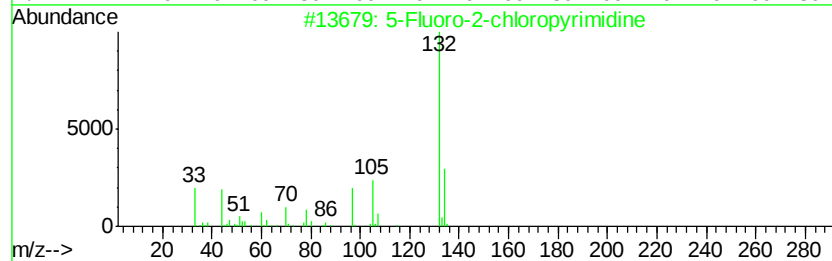
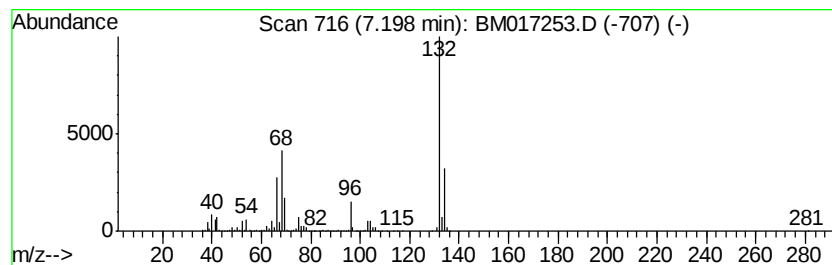
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	86.67 ng	7554960	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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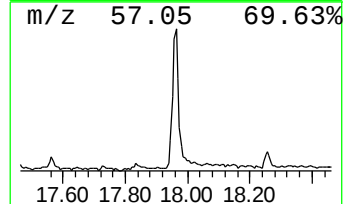
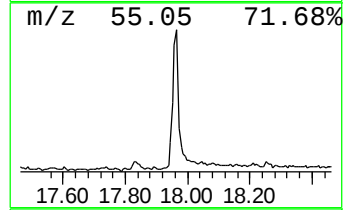
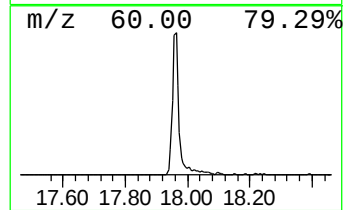
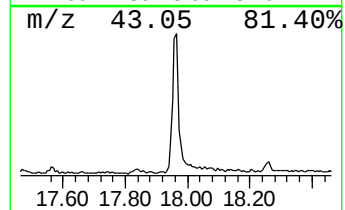
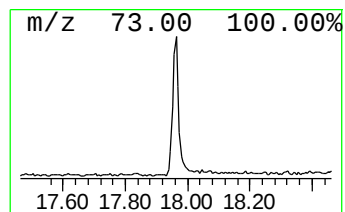
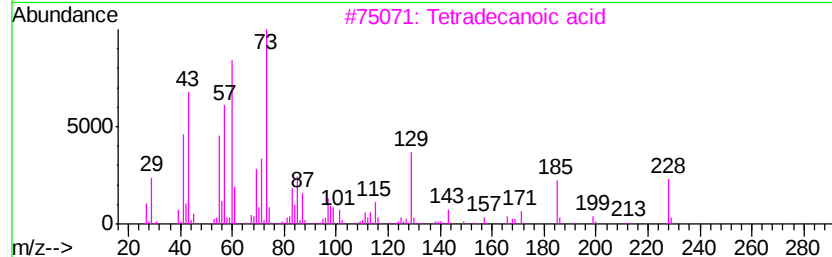
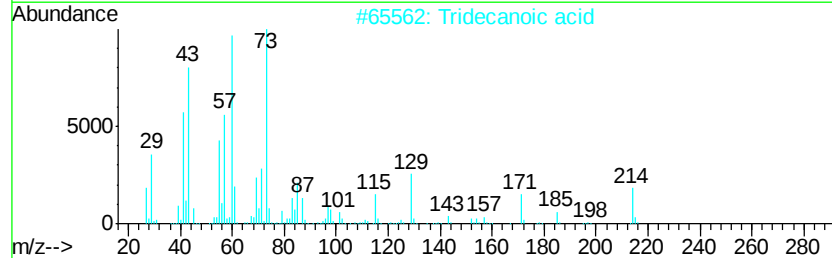
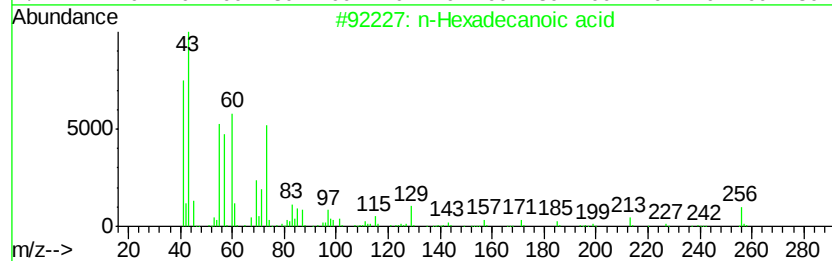
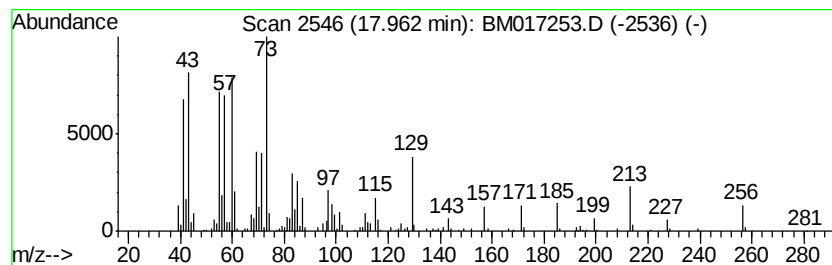
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.96	3.42 ng	664471	Phenanthrene-d10		17.06
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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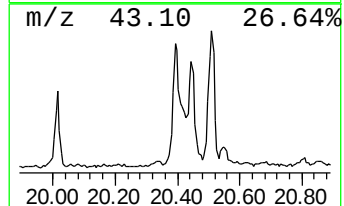
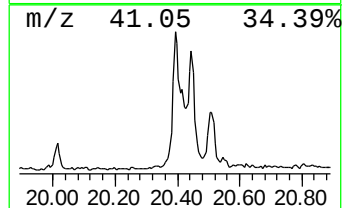
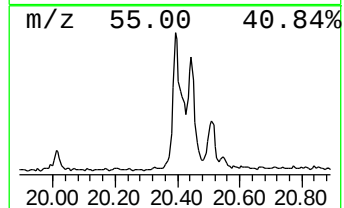
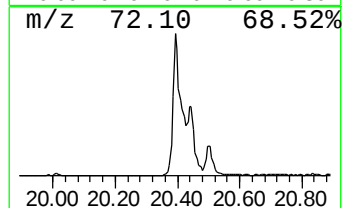
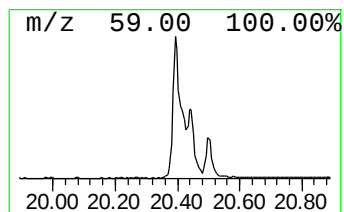
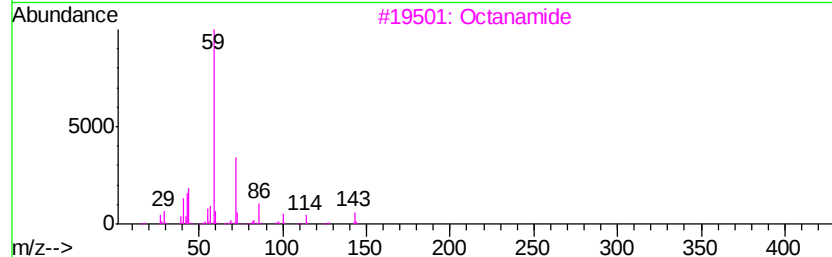
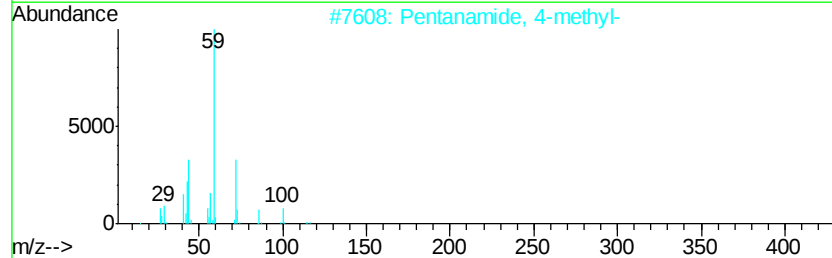
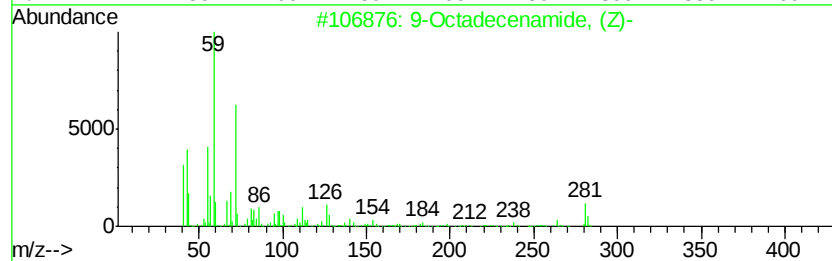
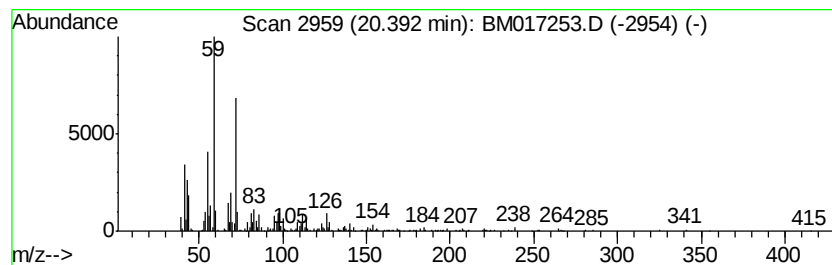
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.39	5.53 ng	1222150	Chrysene-d12	21.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	64
3		Octanamide	143	C8H17NO	000629-01-6	59
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	56
5		7-Nonenamide	155	C9H17NO	090949-53-4	53



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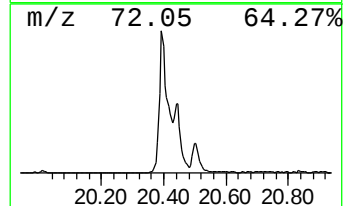
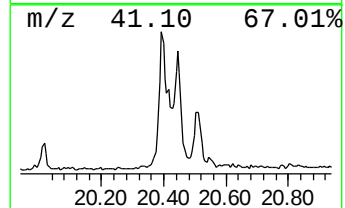
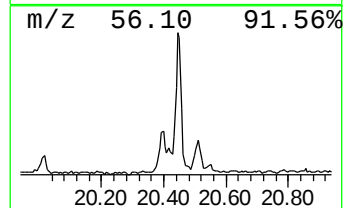
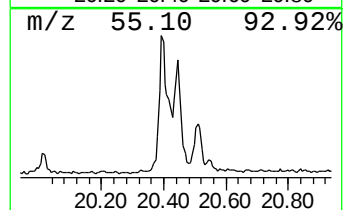
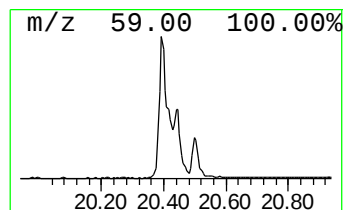
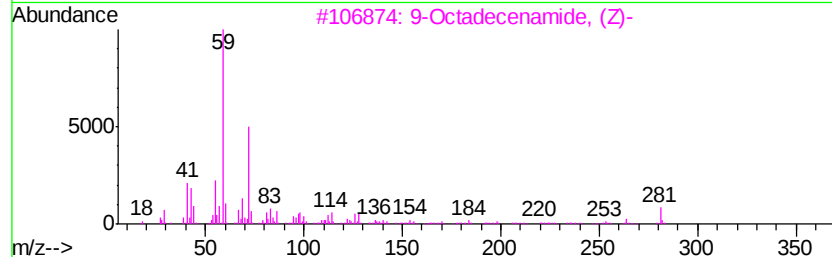
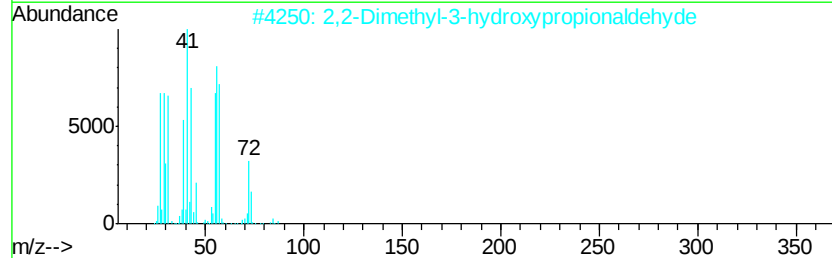
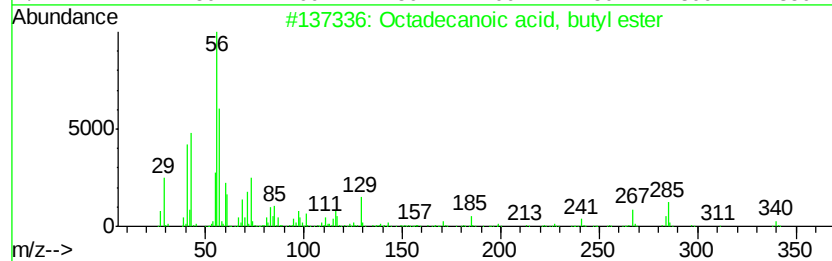
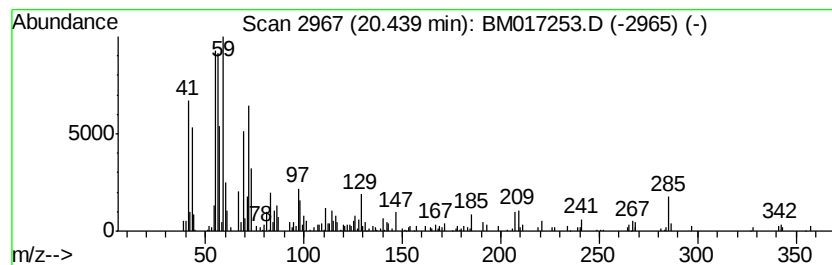
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Peak Number 6 unknown20.44 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.44	3.21 ng	708750	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	46
2		2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	38
3		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	38
4		n-Butyl myristate	284	C18H36O2	000110-36-1	27
5		5-Carbamoyl-pentanoic acid ethyl...	173	C8H15NO3	001190-69-8	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
Data File : BM017253.D
Acq On : 20 Oct 2018 06:37
Operator : MJ/SJ
Sample : J5575-14
Misc :
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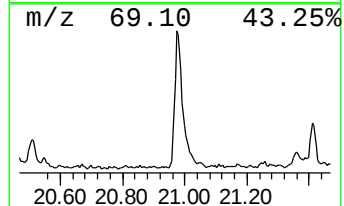
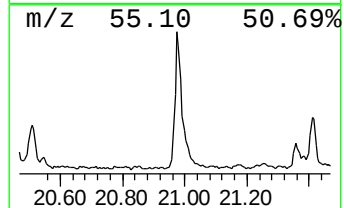
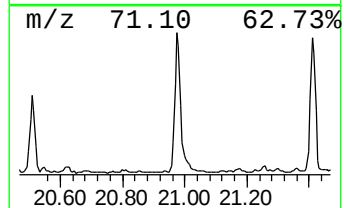
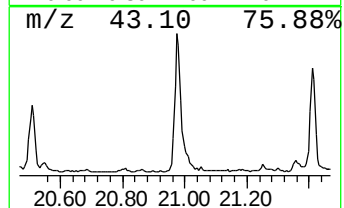
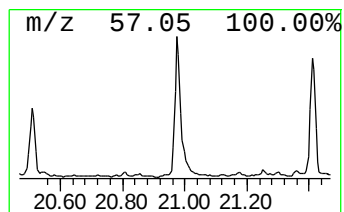
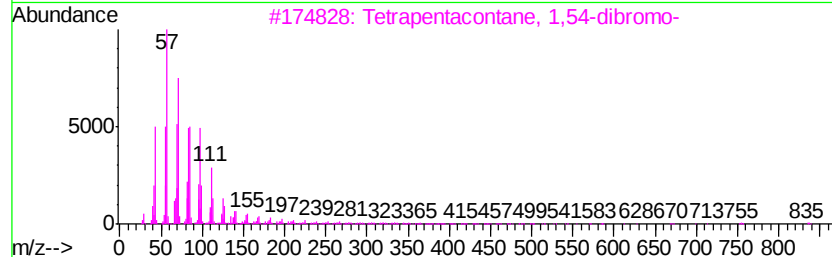
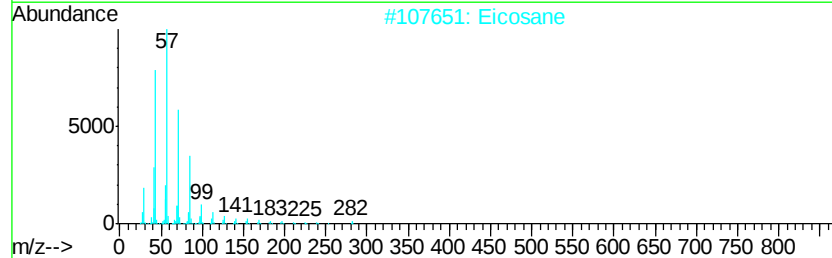
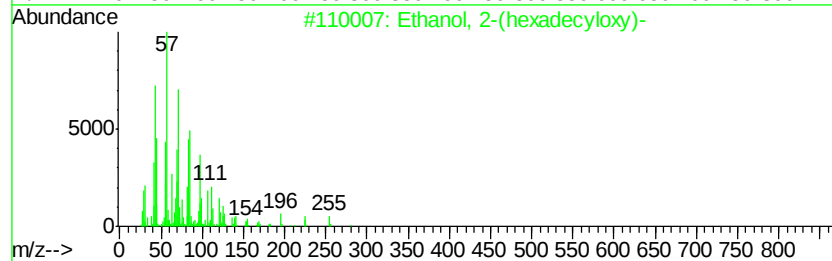
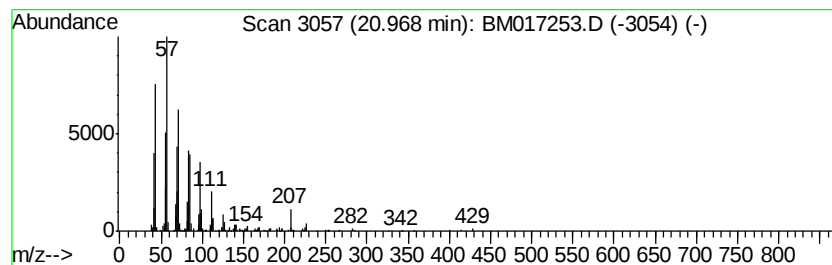
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ClientSampleId :
SSSI-1015-S-DH-25-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Ethanol, 2-(hexadecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.97	4.81 ng	1062680	Chrysene-d12	21.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
2	Eicosane	282	C20H42	000112-95-8	83
3	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	83
4	1-Tricosene	322	C23H46	018835-32-0	70
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
Data File : BM017253.D
Acq On : 20 Oct 2018 06:37
Operator : MJ/SJ
Sample : J5575-14
Misc :
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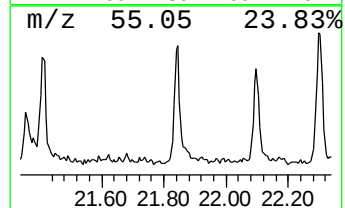
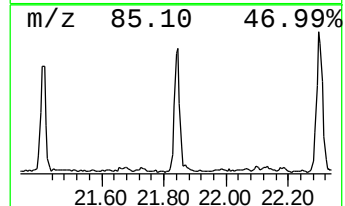
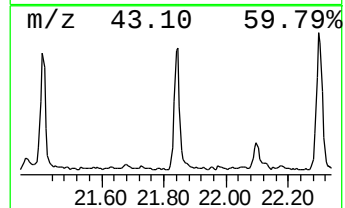
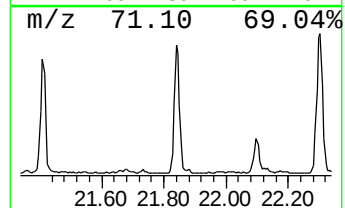
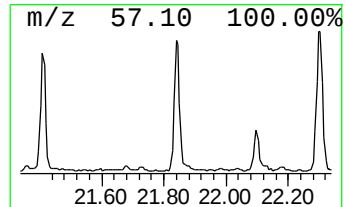
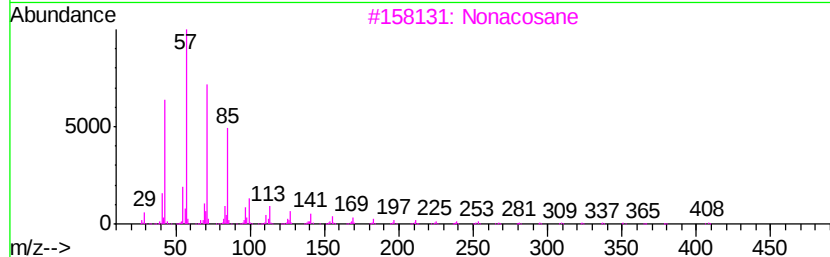
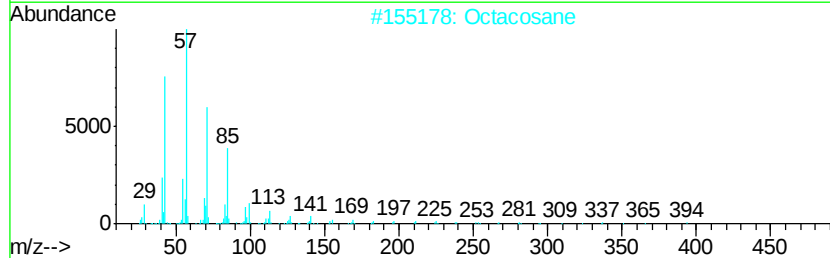
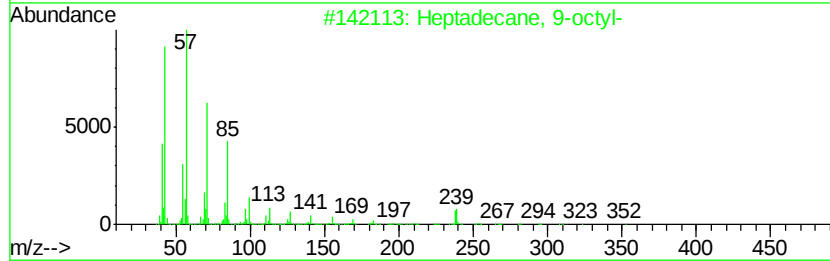
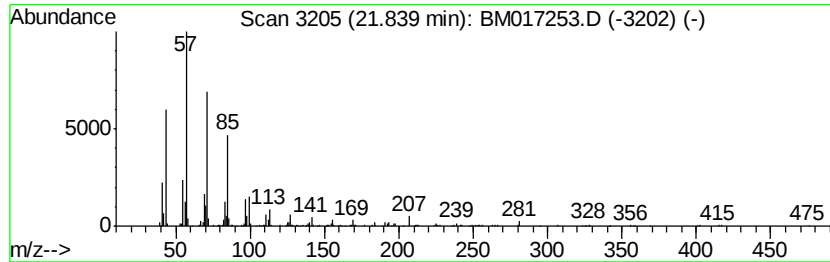
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ClientSampleId :
SSSI-1015-S-DH-25-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	2.28 ng	504556	Chrysene-d12	21.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	90
2	Octacosane	394 C28H58	000630-02-4	90
3	Nonacosane	408 C29H60	000630-03-5	87
4	Octadecane	254 C18H38	000593-45-3	87
5	Heptadecane	240 C17H36	000629-78-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
Data File : BM017253.D
Acq On : 20 Oct 2018 06:37
Operator : MJ/SJ
Sample : J5575-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SSSI-1015-S-DH-25-B

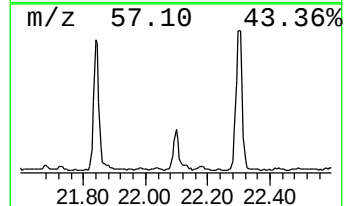
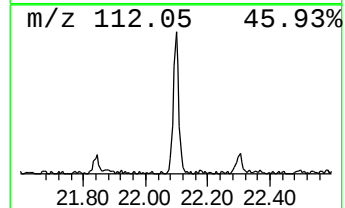
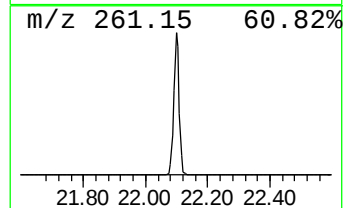
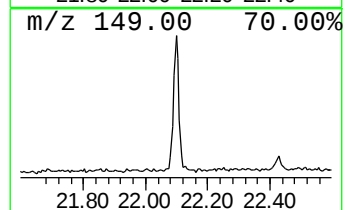
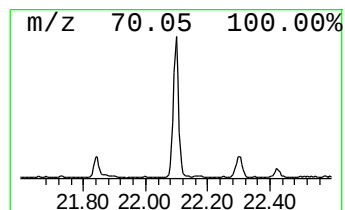
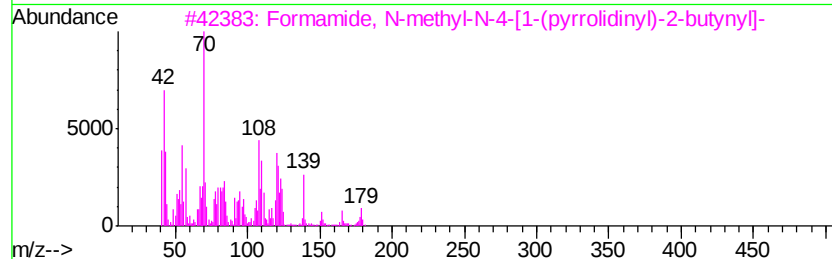
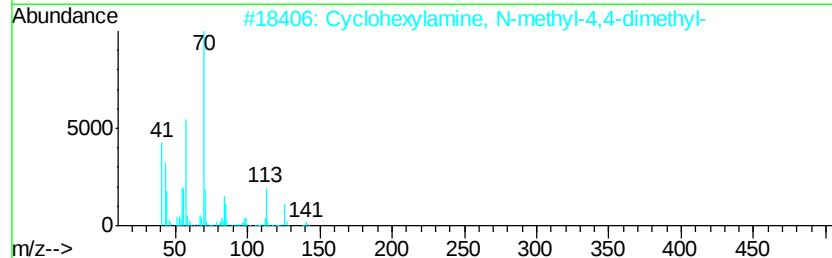
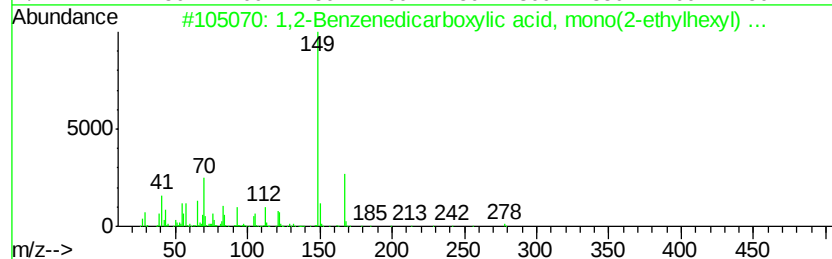
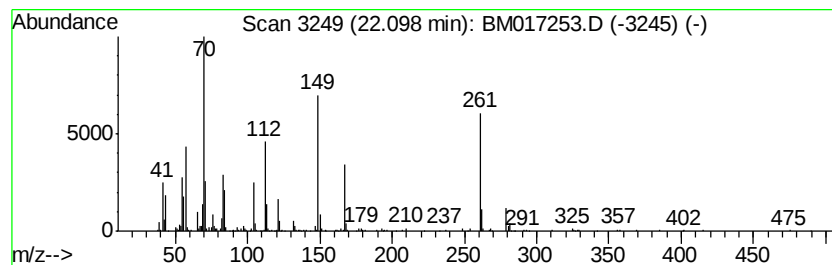
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown22.10 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.10	2.26 ng	499040	Chrysene-d12	21.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Benzenedicarboxylic acid, mo...	278	C16H22O4	004376-20-9	37
2		Cyclohexylamine, N-methyl-4,4-di...	141	C9H19N	045815-91-6	22
3		Formamide, N-methyl-N-4-[1-(pyrr...	180	C10H16N2O	018327-40-7	22
4		Di-n-octyl phthalate	390	C24H38O4	000117-84-0	18
5		3-Chloropropionic acid, 2-ethylh...	220	C11H21ClO2	091369-31-2	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
Data File : BM017253.D
Acq On : 20 Oct 2018 06:37
Operator : MJ/SJ
Sample : J5575-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

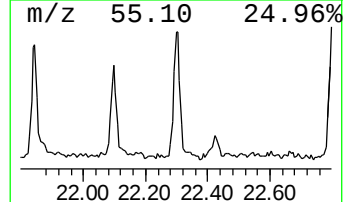
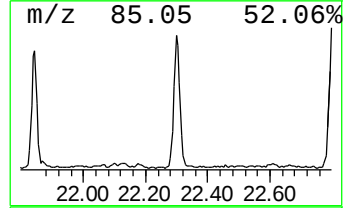
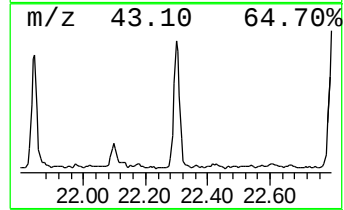
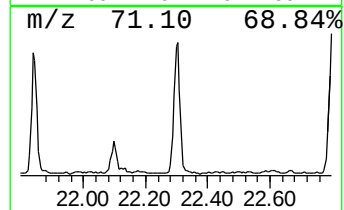
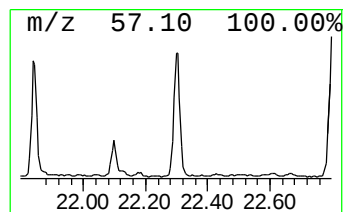
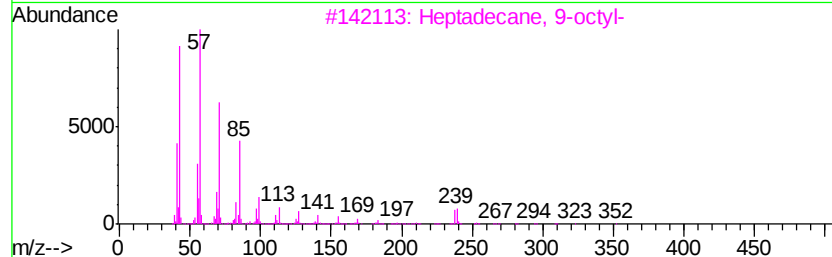
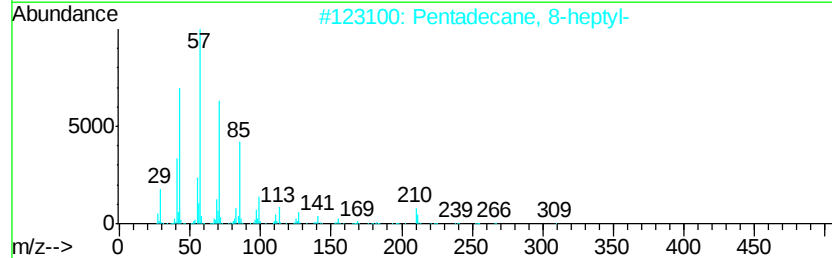
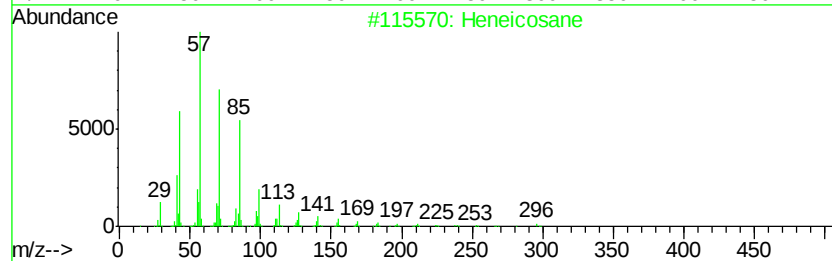
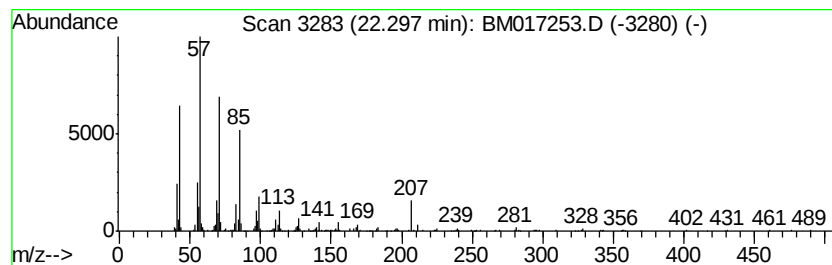
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Pentadecane, 8-heptyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.30	2.75 ng	607475	Chrysene-d12	21.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	87
2	Pentadecane, 8-heptyl-	310 C22H46	071005-15-7	83
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	83
4	Docosane	310 C22H46	000629-97-0	83
5	Triacontane	422 C30H62	000638-68-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
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Operator : MJ/SJ
Sample : J5575-14
Misc :
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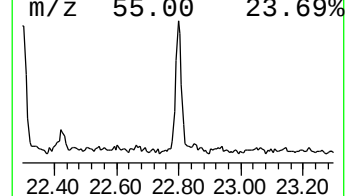
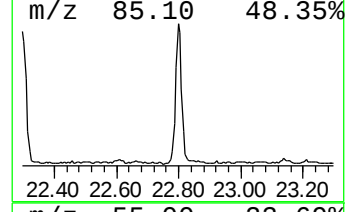
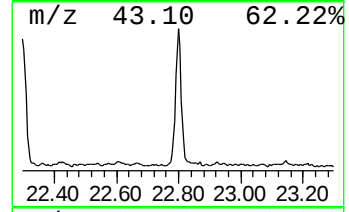
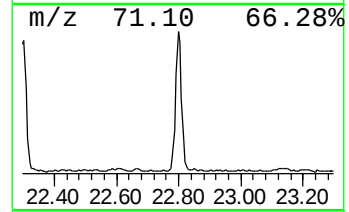
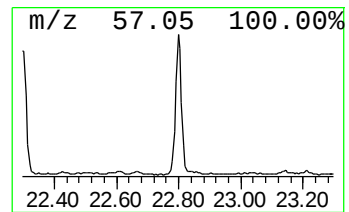
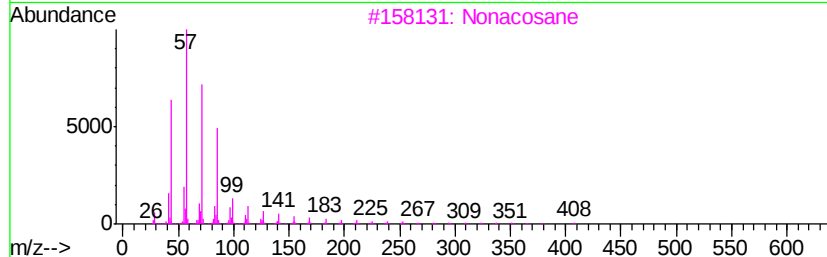
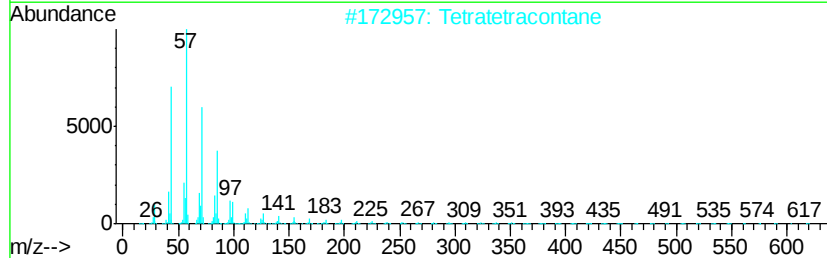
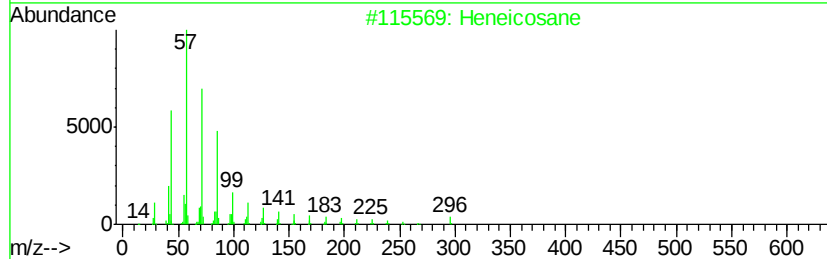
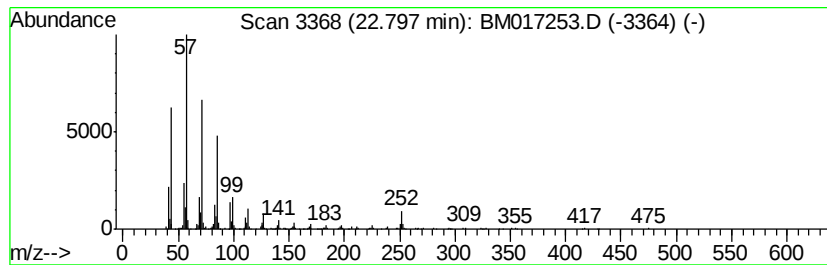
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.80	3.50 ng	668845	Perylene-d12	23.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	97
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Nonacosane	408	C29H60	000630-03-5	83
4	Docosane	310	C22H46	000629-97-0	83
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
Data File : BM017253.D
Acq On : 20 Oct 2018 06:37
Operator : MJ/SJ
Sample : J5575-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

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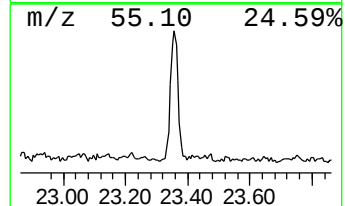
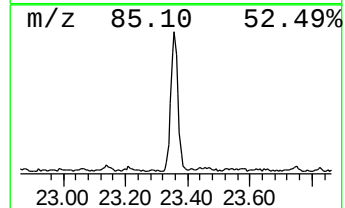
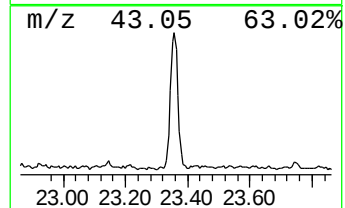
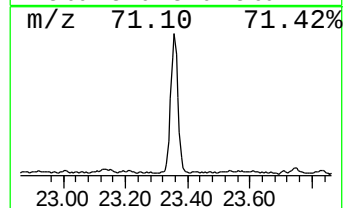
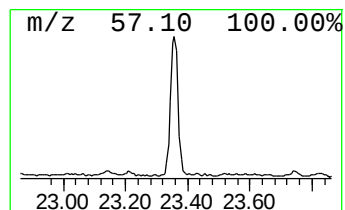
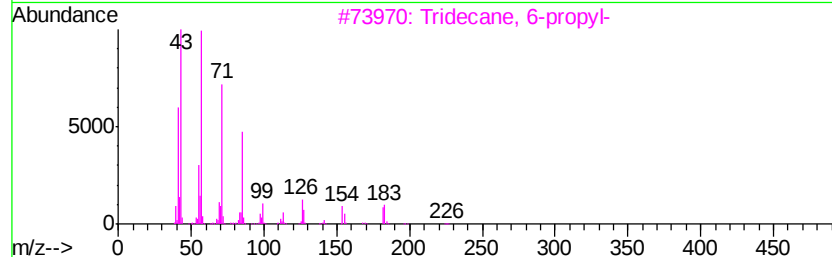
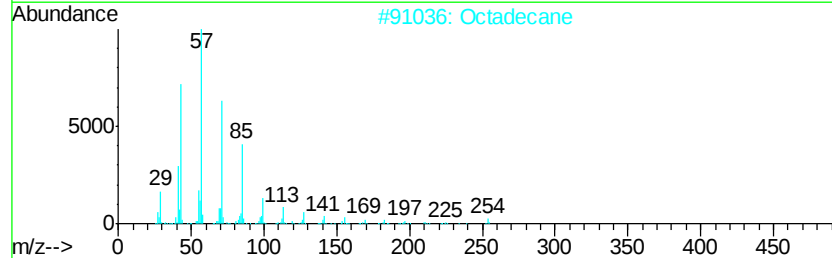
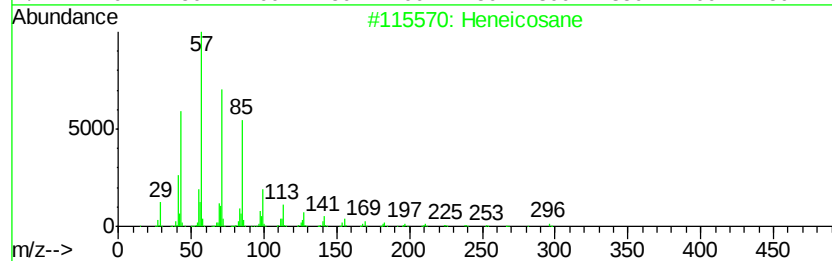
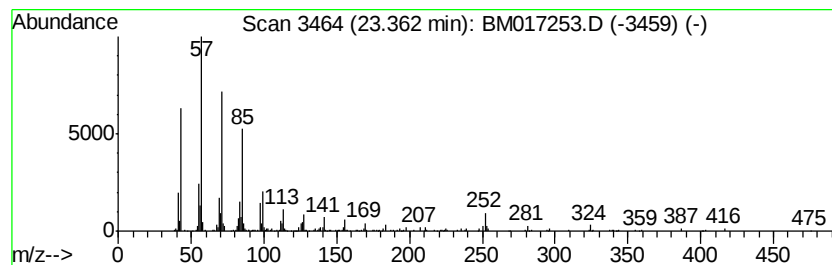
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	3.51 ng	672018	Perylene-d12	23.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	96
2		Octadecane	254	C18H38	000593-45-3	96
3		Tridecane, 6-propyl-	226	C16H34	055045-10-8	90
4		Heptacosane	380	C27H56	000593-49-7	90
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
Data File : BM017253.D
Acq On : 20 Oct 2018 06:37
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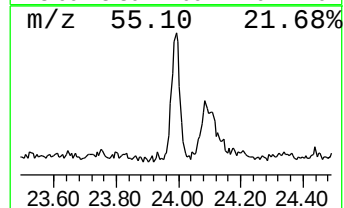
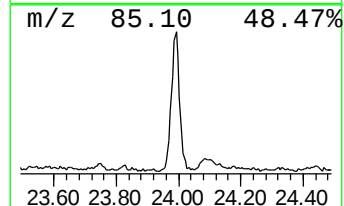
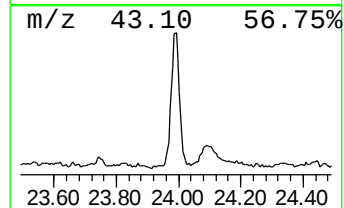
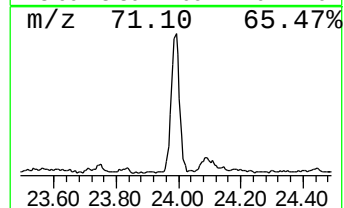
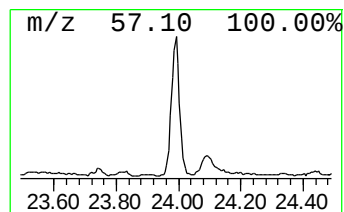
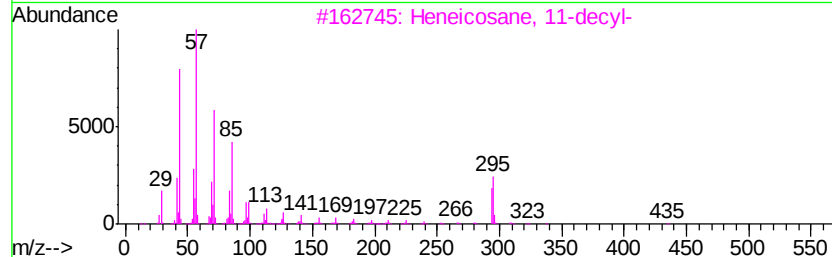
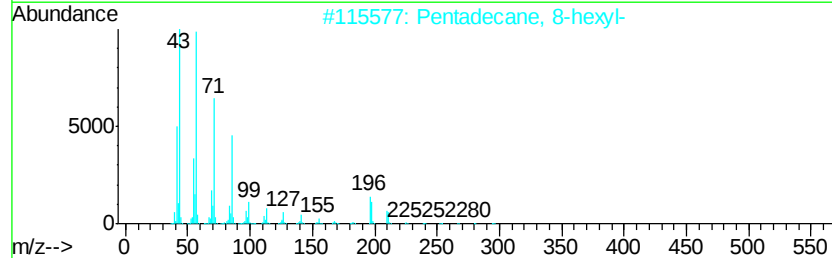
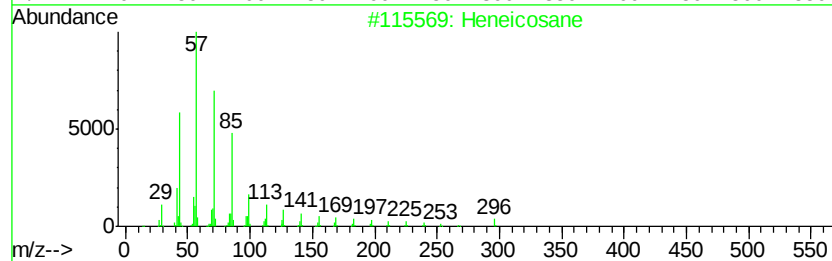
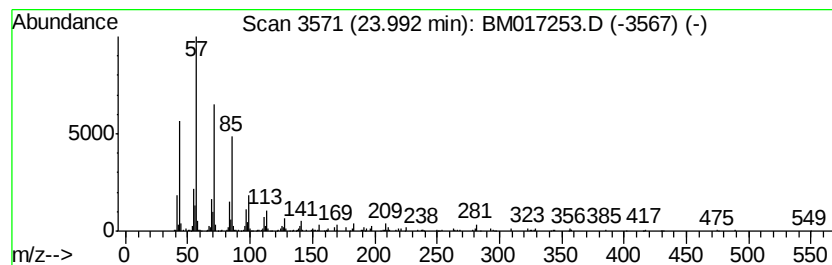
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heneicosane, 11-decyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.57 ng	492057	Perylene-d12	23.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	95
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	90
4		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
5		Eicosane, 10-methyl-	296	C21H44	054833-23-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM101918\
 Data File : BM017253.D
 Acq On : 20 Oct 2018 06:37
 Operator : MJ/SJ
 Sample : J5575-14
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SSSI-1015-S-DH-25-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM101718.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	3.1 ng		271246	1	7.66	1743410	20.0
unknown7.20	7.20	86.7 ng		7554960	1	7.66	1743410	20.0
n-Hexadecanoic acid	17.96	3.4 ng		664471	4	17.06	3890490	20.0
9-Octadecenamide, ...	20.39	5.5 ng		1222150	5	21.25	4419170	20.0
unknown20.44	20.44	3.2 ng		708750	5	21.25	4419170	20.0
Ethanol, 2-(hexad...	20.97	4.8 ng		1062680	5	21.25	4419170	20.0
Heptadecane, 9-oc...	21.84	2.3 ng		504556	5	21.25	4419170	20.0
unknown22.10	22.10	2.3 ng		499040	5	21.25	4419170	20.0
Pentadecane, 8-he...	22.30	2.8 ng		607475	5	21.25	4419170	20.0
Heneicosane	22.80	3.5 ng		668845	6	23.46	3824300	20.0
Octadecane	23.36	3.5 ng		672018	6	23.46	3824300	20.0
Heneicosane, 11-d...	23.99	2.6 ng		492057	6	23.46	3824300	20.0