

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
 Data File : BM010062.D
 Acq On : 16 May 2017 20:27
 Operator : SJ/MA
 Sample : I3171-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WS-4

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

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

Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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	4.287	199	204	218	rBV	1169295	1592914	26.69%	6.015%
2	4.893	301	307	320	rBV	1870888	2516457	42.16%	9.503%
3	5.346	379	384	399	rBV	462726	722515	12.11%	2.728%
4	5.946	481	486	496	rBV	297400	448056	7.51%	1.692%
5	6.940	649	655	667	rBV	290072	518188	8.68%	1.957%
6	7.287	708	714	728	rVB	826935	1349885	22.62%	5.098%
7	7.751	786	793	801	rBV2	206890	345012	5.78%	1.303%
8	8.069	841	847	859	rBV	1059144	1683040	28.20%	6.356%
9	8.928	983	993	1006	rBV	998923	1703625	28.54%	6.433%
10	10.551	1263	1269	1282	rVB	241778	441396	7.40%	1.667%
11	13.022	1682	1689	1698	rBV	2146066	3160586	52.95%	11.935%
12	14.410	1916	1925	1934	rBV2	360151	561729	9.41%	2.121%
13	15.910	2173	2180	2193	rBV	1254885	1924912	32.25%	7.269%
14	17.163	2387	2393	2402	rBV	498968	785930	13.17%	2.968%
15	18.039	2538	2542	2549	rBV2	141512	185794	3.11%	0.702%
16	19.321	2756	2760	2768	rBV3	120693	179059	3.00%	0.676%
17	19.786	2834	2839	2845	rBV	4832318	5968462	100.00%	22.539%
18	21.045	3050	3053	3060	rBV8	79956	117689	1.97%	0.444%
19	21.351	3101	3105	3113	rVB	730555	982275	16.46%	3.709%
20	22.497	3296	3300	3307	rVB	325879	451744	7.57%	1.706%
21	23.644	3489	3495	3506	rVB	396144	841639	14.10%	3.178%

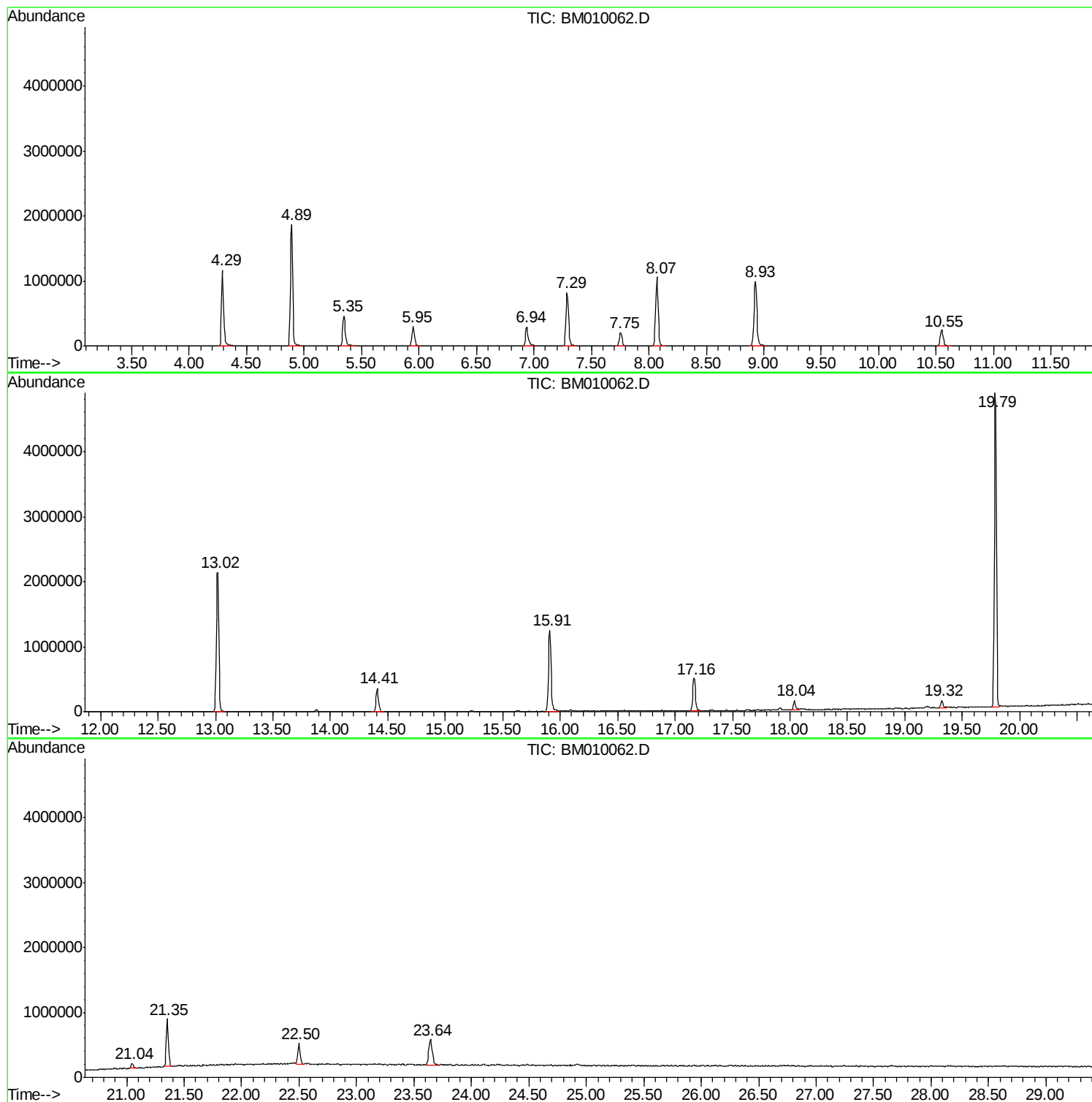
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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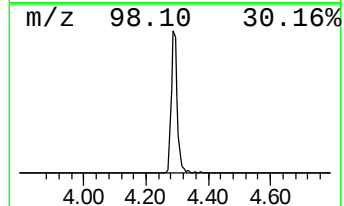
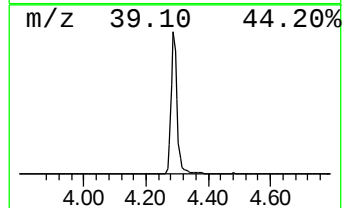
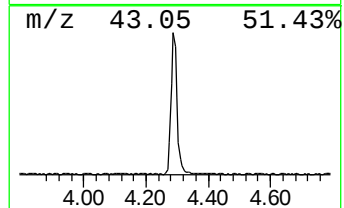
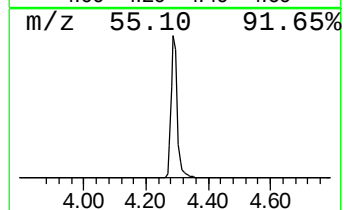
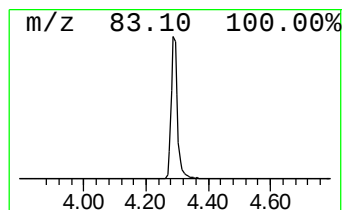
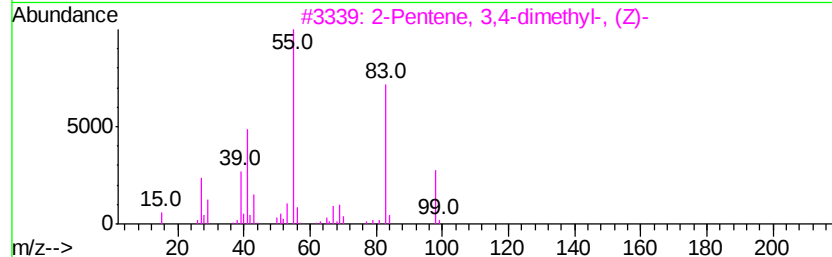
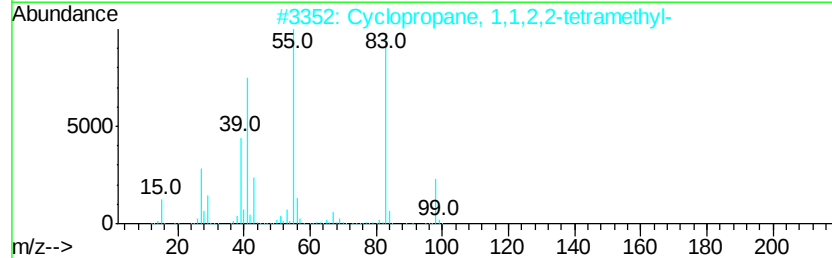
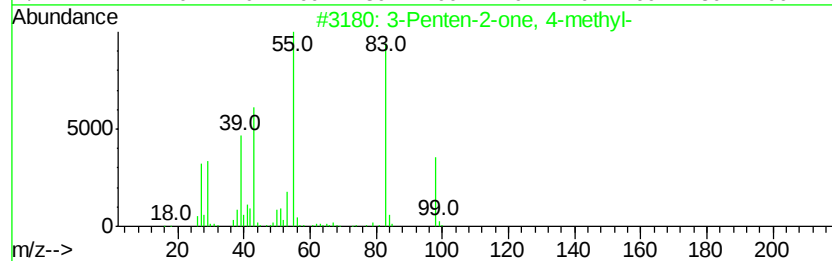
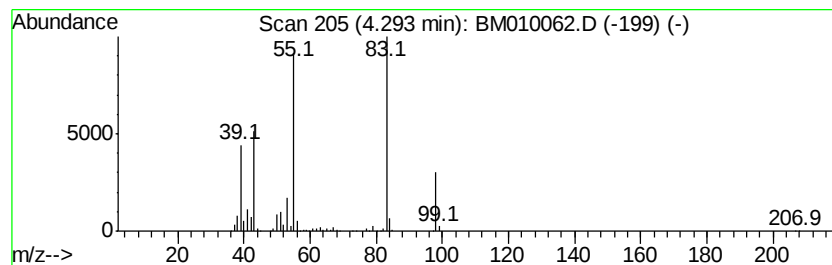
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	92.34 ng	1592910	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	81
2		Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	80
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	53
4		3-Hexen-2-one	98	C6H10O	000763-93-9	52
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	50



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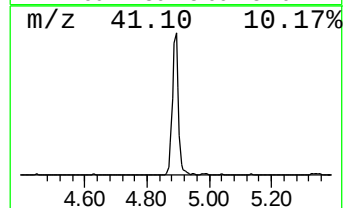
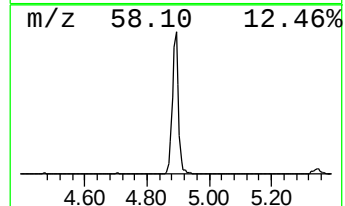
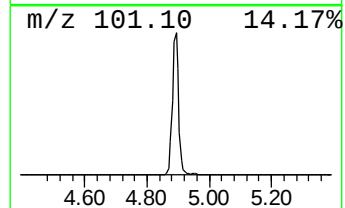
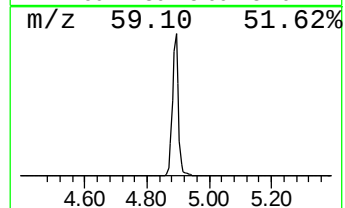
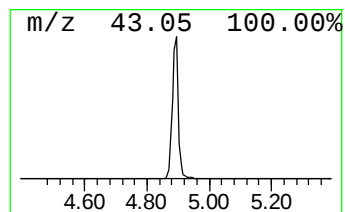
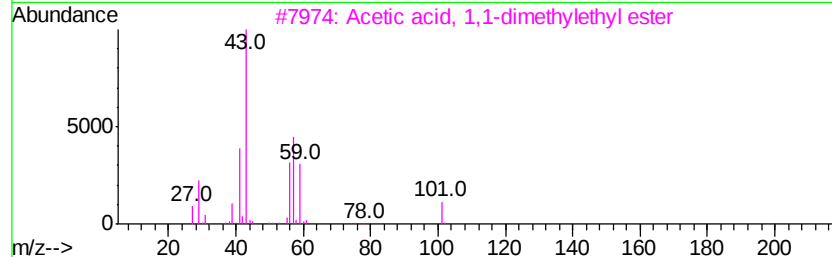
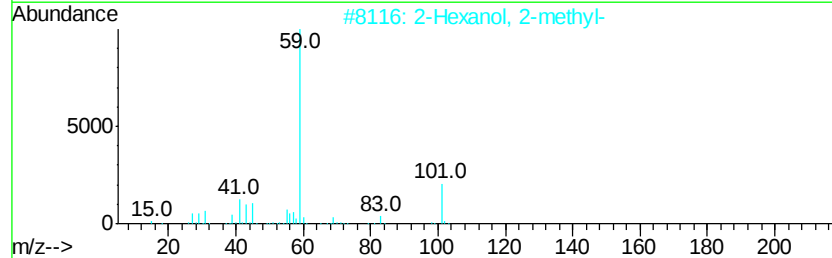
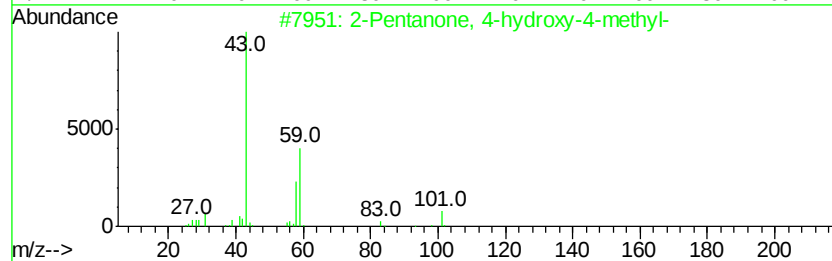
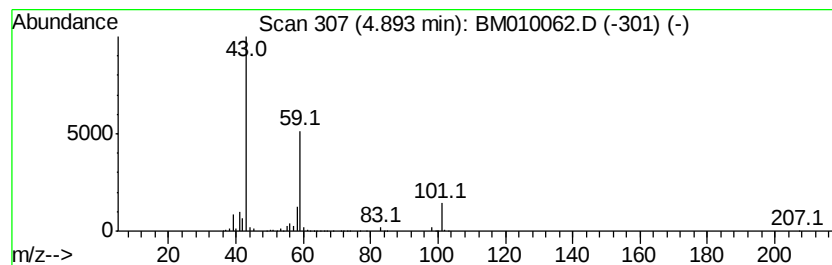
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	145.88 ng	2516460	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
5		1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23



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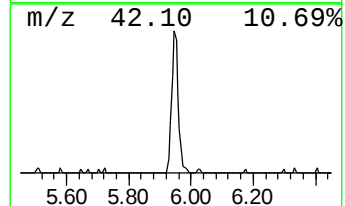
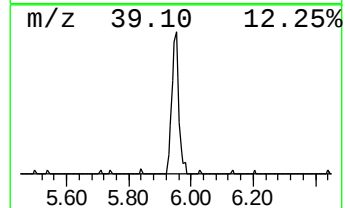
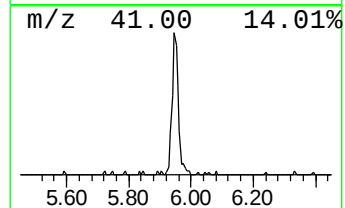
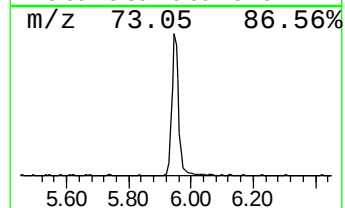
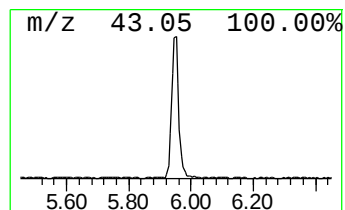
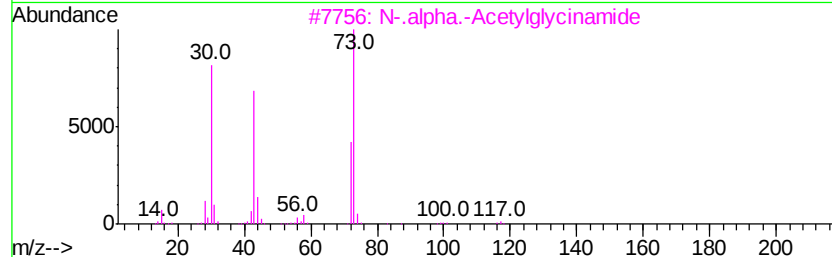
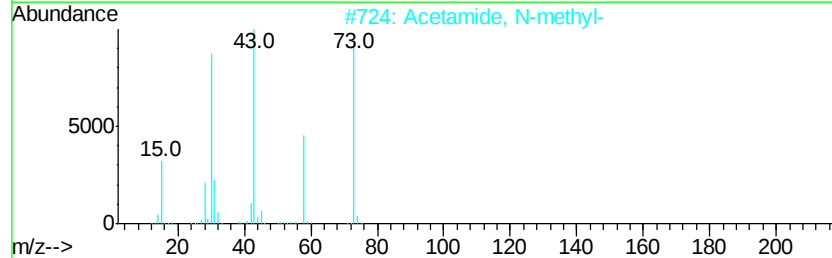
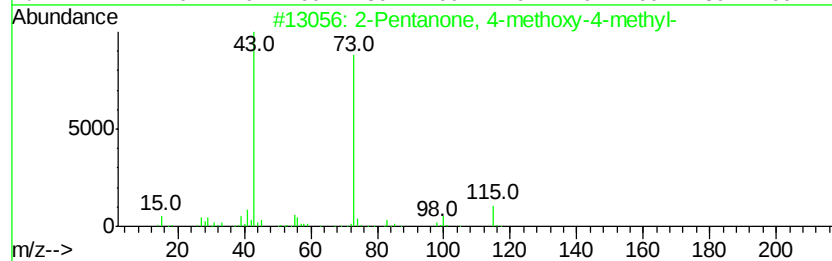
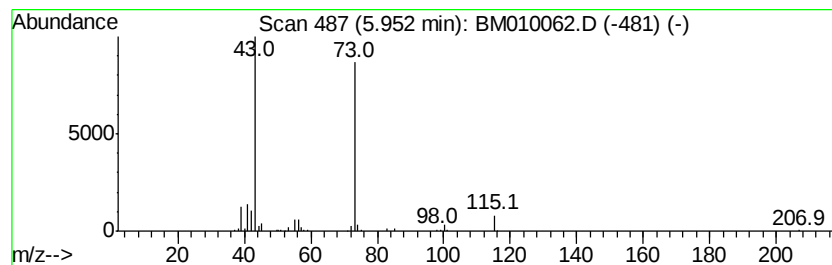
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	25.97 ng	448056	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	59
3		N-.alpha.-Acetylglucosinamide	116	C4H8N2O2	002620-63-5	25
4		N-Ethylformamide	73	C3H7NO	000627-45-2	23
5		2-Heptanone	114	C7H14O	000110-43-0	17



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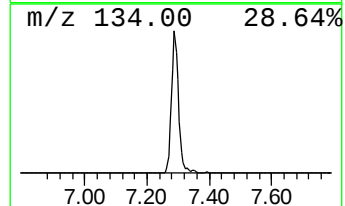
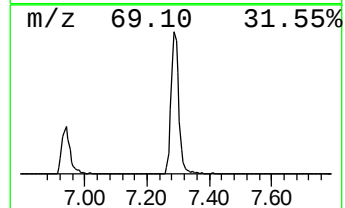
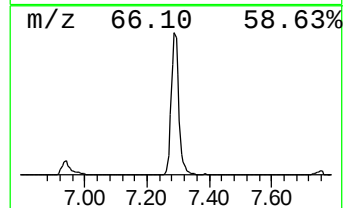
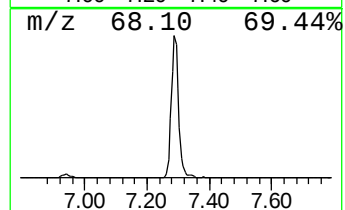
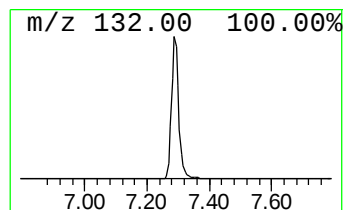
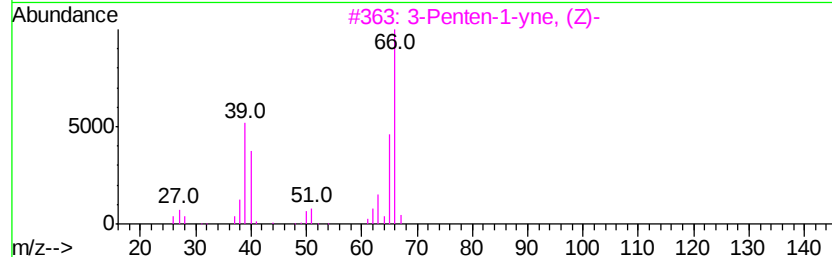
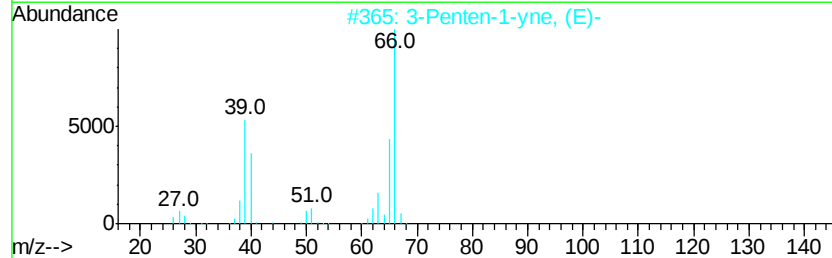
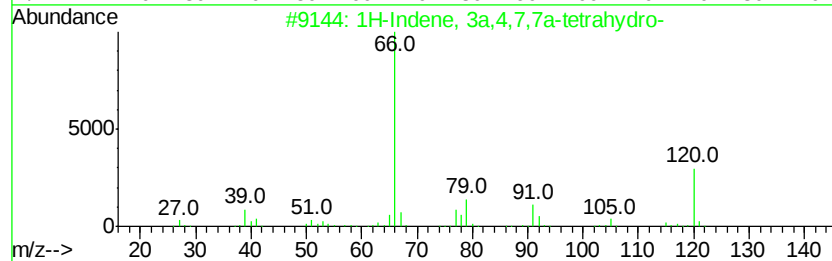
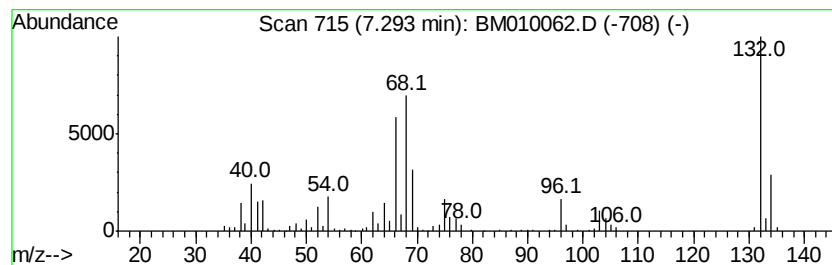
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown7.29 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	78.25 ng	1349890	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 3a,4,7,7a-tetrahydro-	120	C9H12	003048-65-5	27
2		3-Penten-1-yne, (E)-	66	C5H6	002004-69-5	27
3		3-Penten-1-yne, (Z)-	66	C5H6	001574-40-9	27
4		1-Penten-3-yne	66	C5H6	000646-05-9	27
5		2,4-Hexadienenitrile	93	C6H7N	001516-01-4	25



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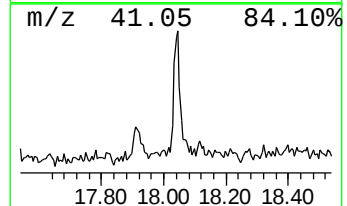
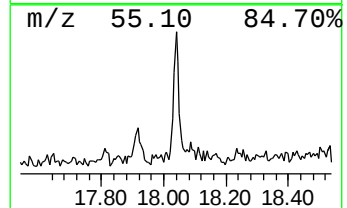
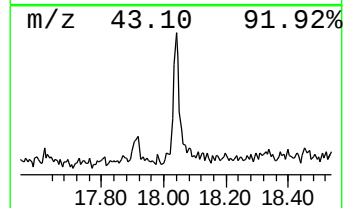
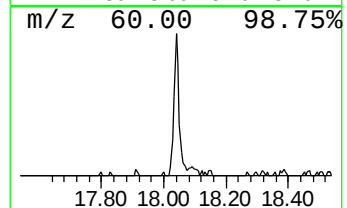
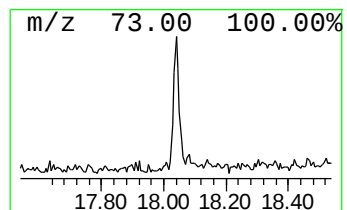
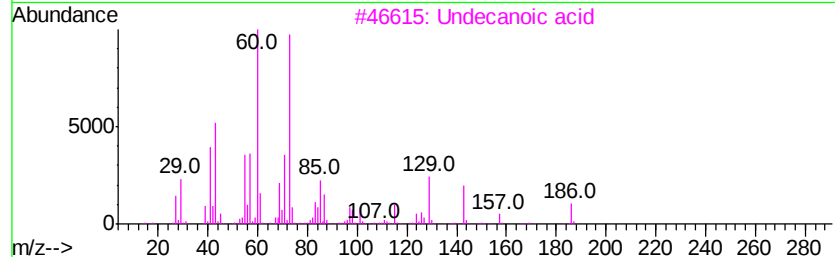
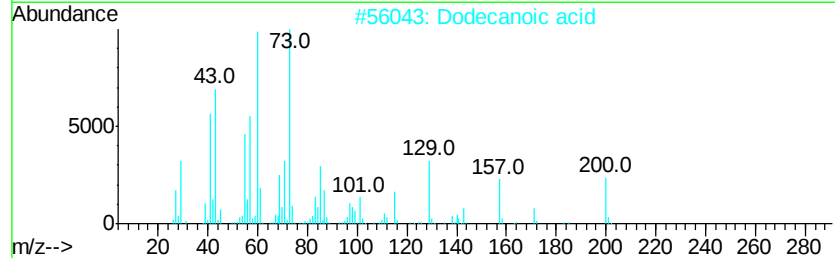
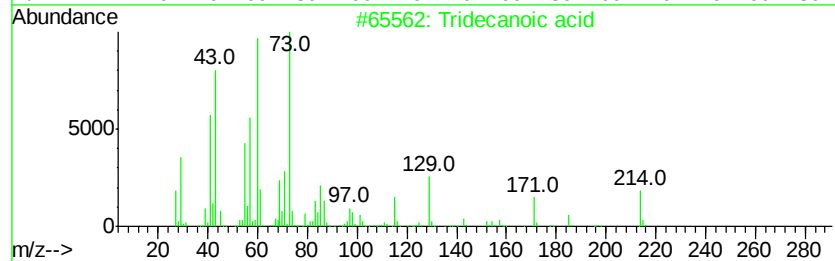
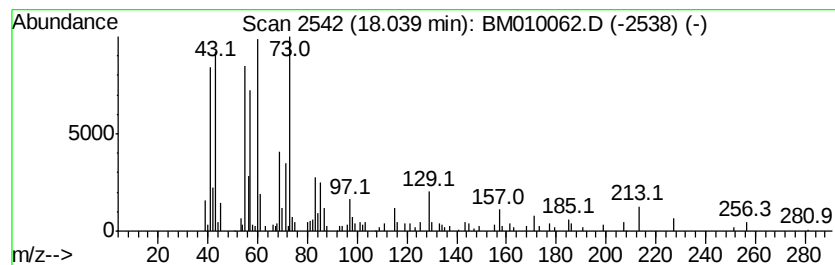
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.04	4.73 ng	185794	Phenanthrene-d10	17.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	80
2	Dodecanoic acid	200	C12H24O2	000143-07-7	78
3	Undecanoic acid	186	C11H22O2	000112-37-8	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	59



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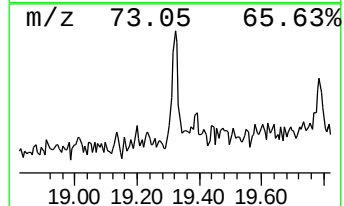
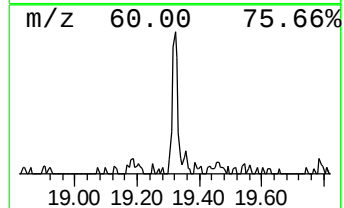
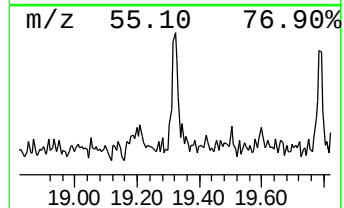
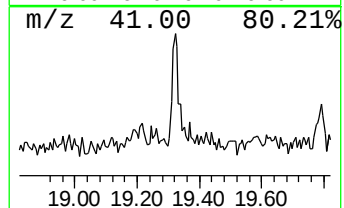
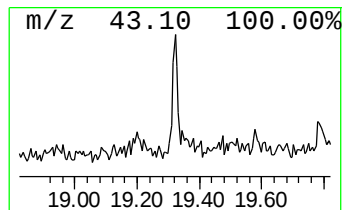
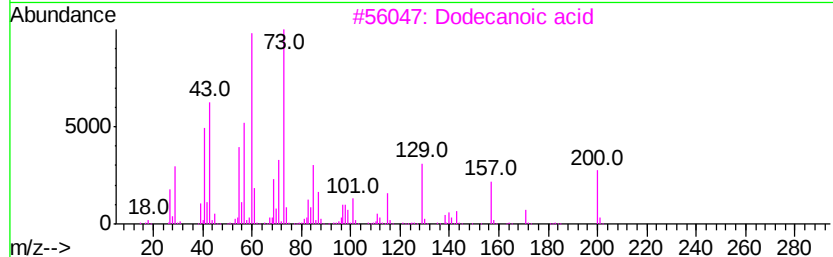
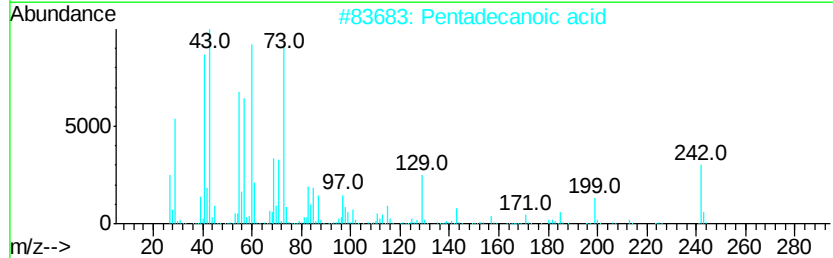
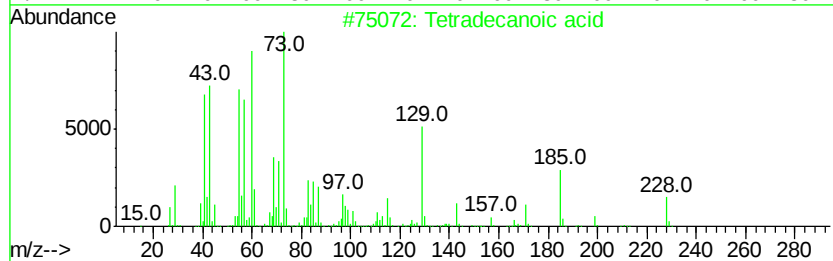
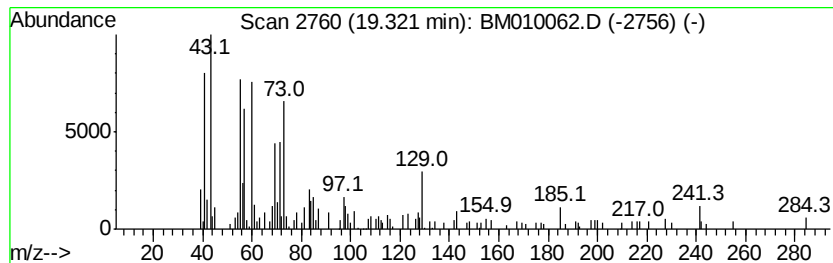
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.32	3.65 ng	179059	Chrysene-d12	21.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
3	Dodecanoic acid	200	C12H24O2	000143-07-7	46
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Heptanoic acid	130	C7H14O2	000111-14-8	38



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010062.D
Acq On : 16 May 2017 20:27
Operator : SJ/MA
Sample : I3171-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

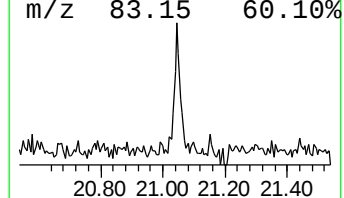
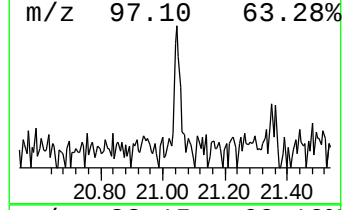
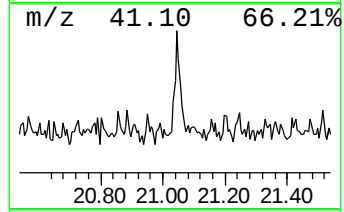
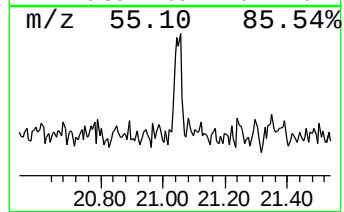
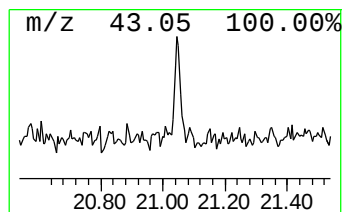
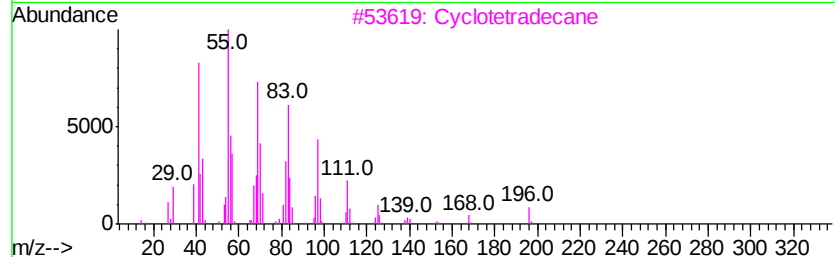
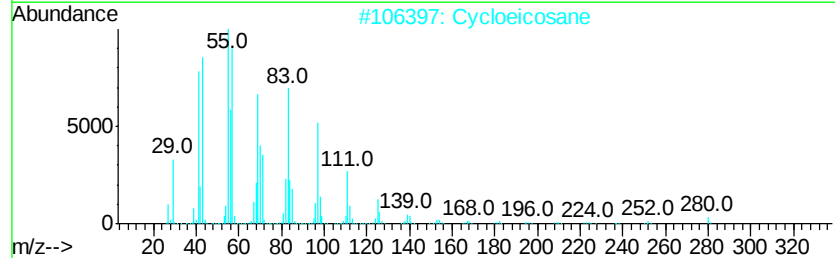
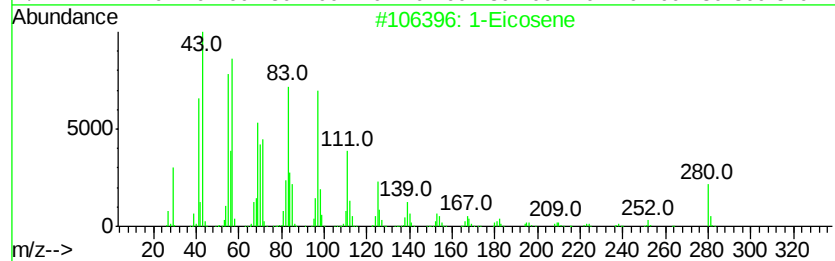
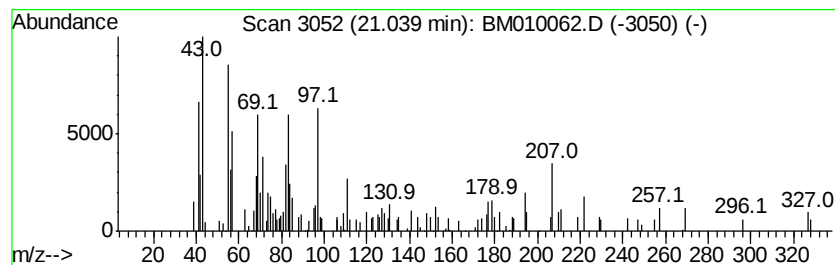
Instrument :
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ClientSampleId :
WS-4

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Eicosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.04	2.40 ng	117689	Chrysene-d12	21.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Eicosene		280 C20H40	003452-07-1 70
2	Cycloeicosane		280 C20H40	000296-56-0 70
3	Cyclotetradecane		196 C14H28	000295-17-0 64
4	17-Pentatriacontene		491 C35H70	006971-40-0 62
5	Trichloroacetic acid, pentadecyl...		372 C17H31Cl3O2	074339-53-0 58



Data Path : Z:\HPCHEM1\BNA M\DATA\BM051617\
Data File : BM010062.D
Acq On : 16 May 2017 20:27
Operator : SJ/MA
Sample : I3171-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WS-4

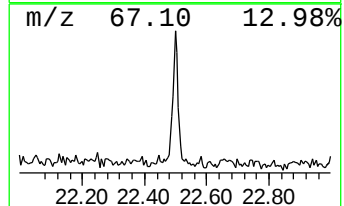
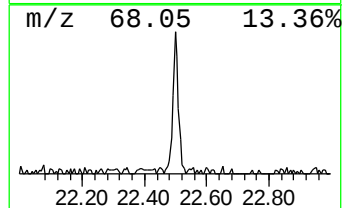
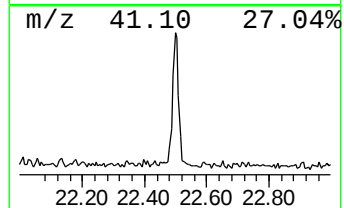
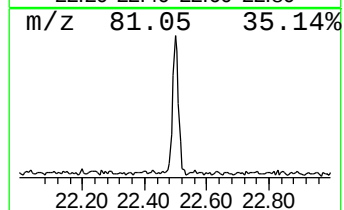
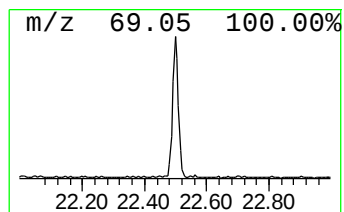
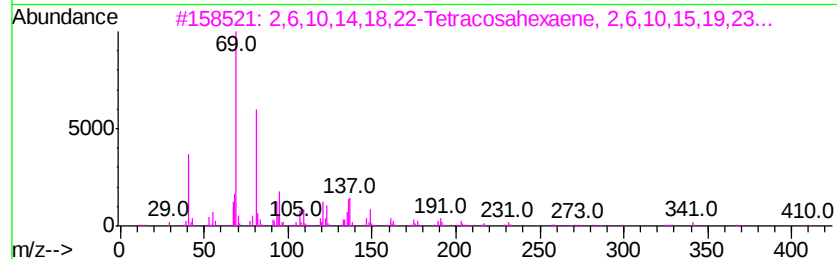
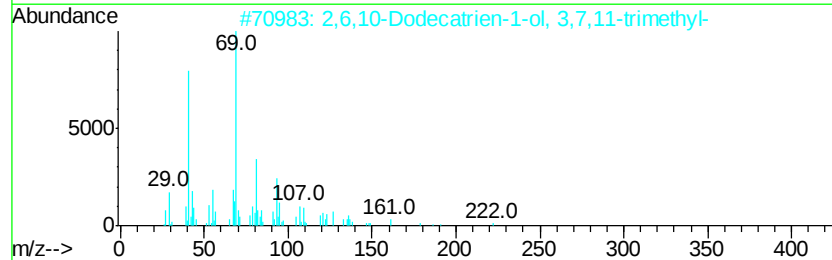
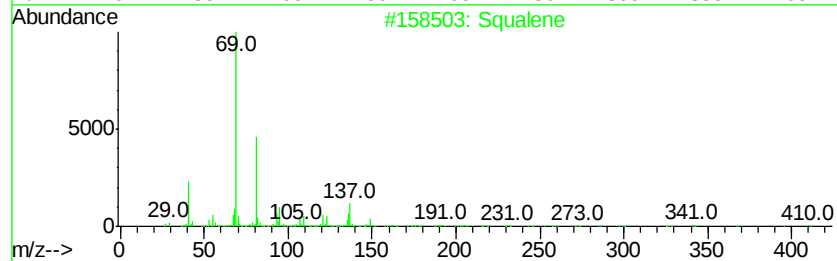
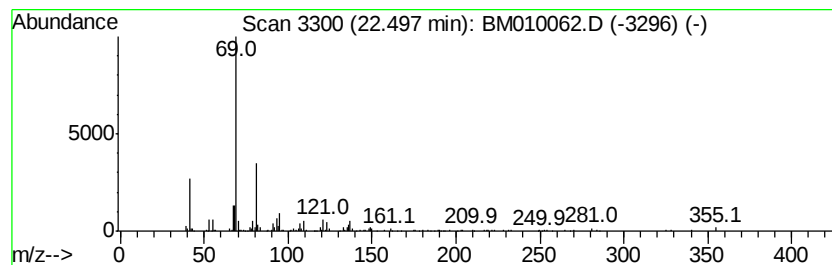
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	10.73 ng	451744	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	83
2		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
3		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	64
4		.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O5	1000154-77-2	56
5		2,6-Octadiene, 4-methyl-	124	C9H16	074498-94-5	53



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM051617\
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Acq On : 16 May 2017 20:27
Operator : SJ/MA
Sample : I3171-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
WS-4

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\8270-BM051117.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
3-Penten-2-one, 4...	4.29	92.3	ng	1592910	1	7.76	345012	20.0
2-Pentanone, 4-hy...	4.89	145.9	ng	2516460	1	7.76	345012	20.0
2-Pentanone, 4-me...	5.95	26.0	ng	448056	1	7.76	345012	20.0
unknown7.29	7.29	78.3	ng	1349890	1	7.76	345012	20.0
Tridecanoic acid	18.04	4.7	ng	185794	4	17.16	785930	20.0
Tetradecanoic acid	19.32	3.6	ng	179059	5	21.35	982275	20.0
1-Eicosene	21.04	2.4	ng	117689	5	21.35	982275	20.0
Squalene	22.50	10.7	ng	451744	6	23.64	841639	20.0