

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
 Data File : BM018640.D
 Acq On : 18 Jan 2019 17:01
 Operator : JU/SJ
 Sample : K1173-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RBR-200050

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-BM010919.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	3.516	69	73	84	rBV	179351	278388	2.81%	0.304%
2	4.281	199	203	211	rBV	71424	100480	1.01%	0.110%
3	4.881	300	305	313	rVB	197912	282132	2.85%	0.308%
4	5.328	374	381	396	rBV	3802723	5410603	54.58%	5.906%
5	6.910	642	650	660	rBV	3551040	5540940	55.90%	6.049%
6	7.269	704	711	722	rBV	3950079	6177573	62.32%	6.743%
7	7.734	783	790	798	rBV	919108	1440155	14.53%	1.572%
8	8.051	837	844	852	rBV	2874865	4559333	45.99%	4.977%
9	8.904	980	989	1001	rBV	2139952	3592020	36.24%	3.921%
10	10.528	1256	1265	1276	rBV	1063240	1821935	18.38%	1.989%
11	12.998	1678	1685	1696	rBV	4914143	7180370	72.43%	7.838%
12	13.845	1823	1829	1836	rBV	465427	667318	6.73%	0.728%
13	14.257	1892	1899	1909	rBV4	46702	135210	1.36%	0.148%
14	14.386	1914	1921	1931	rBV2	1421758	2239129	22.59%	2.444%
15	15.880	2168	2175	2193	rBV	4143997	6097659	61.51%	6.656%
16	17.133	2381	2388	2400	rBV2	1801456	2677447	27.01%	2.923%
17	18.021	2534	2539	2549	rBV	1031971	1637061	16.51%	1.787%
18	18.098	2549	2552	2563	rVB	93466	203247	2.05%	0.222%
19	19.304	2753	2757	2774	rBV	353837	628632	6.34%	0.686%
20	19.768	2830	2836	2846	rBV	8199322	9912854	100.00%	10.821%
21	20.562	2968	2971	2975	rBV	93641	105205	1.06%	0.115%
22	21.027	3046	3050	3057	rBV	601163	738376	7.45%	0.806%
23	21.327	3096	3101	3112	rBV	2586033	3298023	33.27%	3.600%
24	21.468	3121	3125	3132	rBV2	425547	509036	5.14%	0.556%
25	21.903	3195	3199	3205	rBV	1325507	1541417	15.55%	1.683%
26	22.374	3274	3279	3292	rVB	2524780	3383250	34.13%	3.693%
27	22.886	3360	3366	3382	rVB	3024747	4941984	49.85%	5.395%
28	23.462	3457	3464	3472	rBV	3272580	5490121	55.38%	5.993%
29	23.597	3481	3487	3500	rVB2	1635133	3246100	32.75%	3.543%
30	24.115	3568	3575	3585	rBV	2375677	4591895	46.32%	5.013%
31	24.874	3697	3704	3713	rBV	1072607	2469637	24.91%	2.696%
32	25.762	3851	3855	3865	rVB3	303657	710388	7.17%	0.775%

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

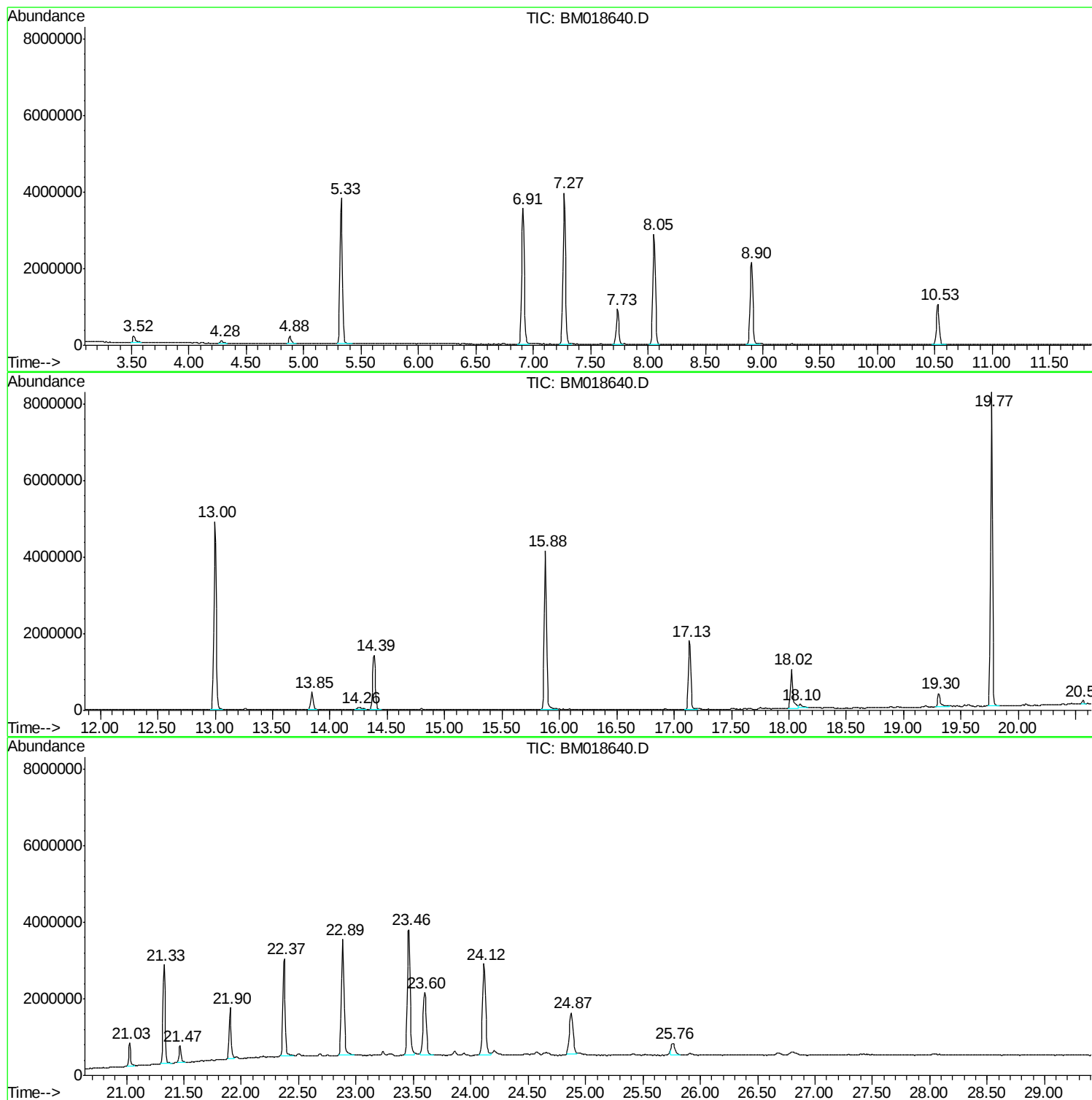
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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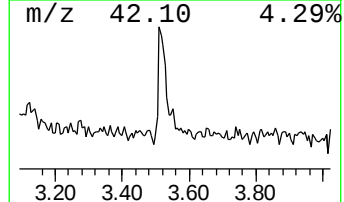
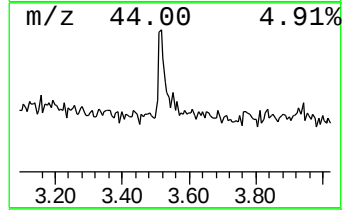
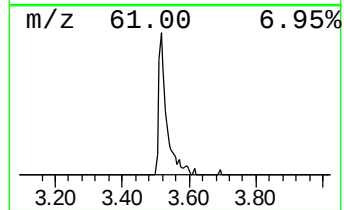
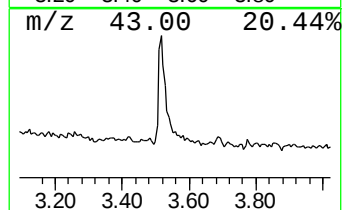
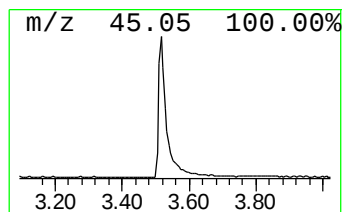
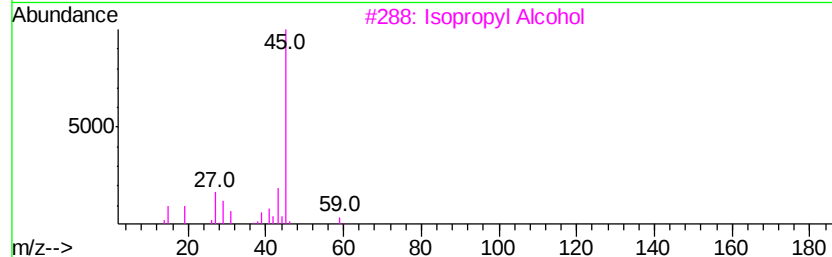
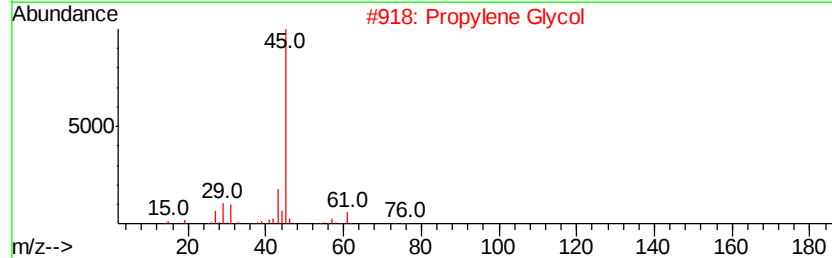
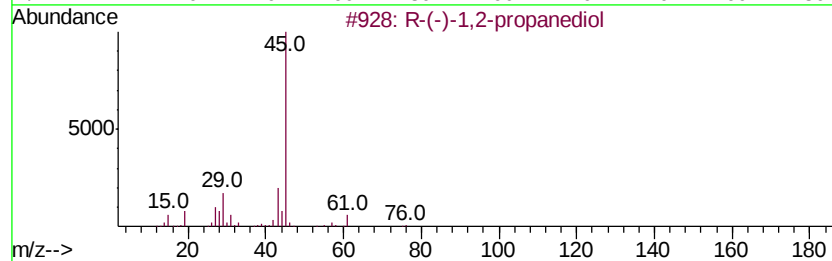
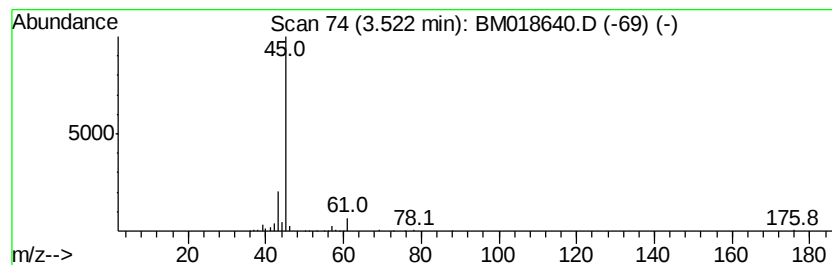
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.52	3.87 ng	278388	1,4-Dichlorobenzene-d4	7.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
2		Propylene Glycol	76	C3H8O2	000057-55-6	78
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	10
5		2-Heptanol, (S)-	116	C7H16O	006033-23-4	9



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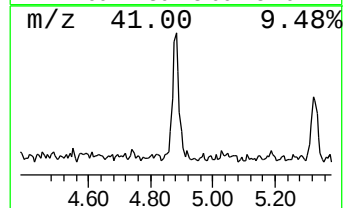
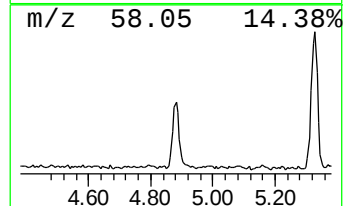
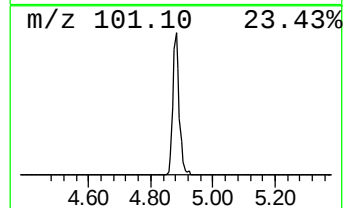
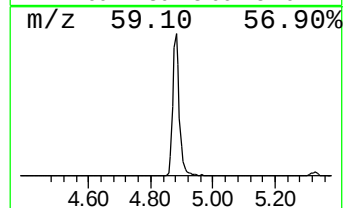
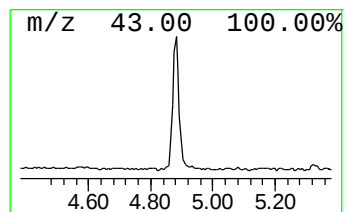
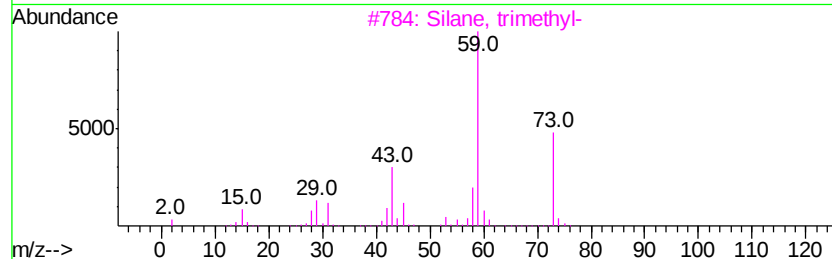
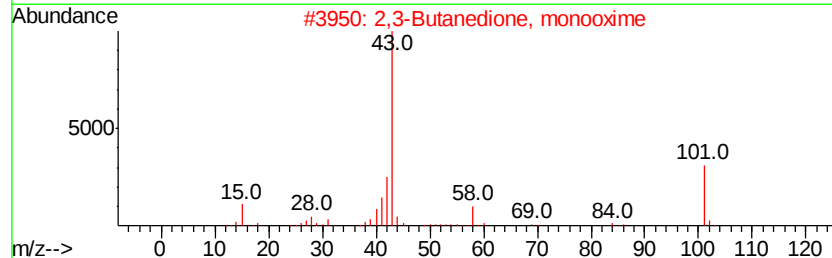
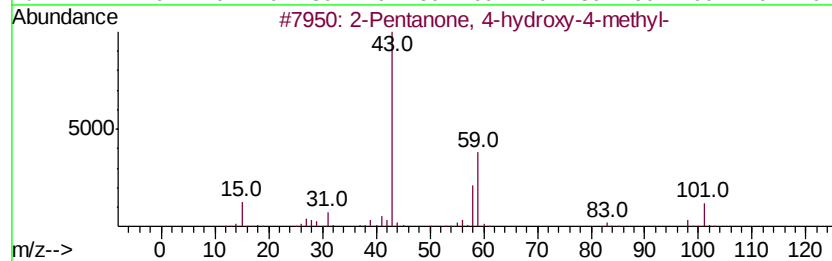
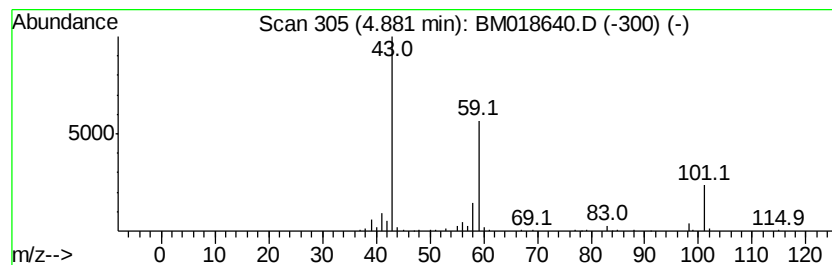
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.88 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	3.92 ng	282132	1,4-Dichlorobenzene-d4	7.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	9		



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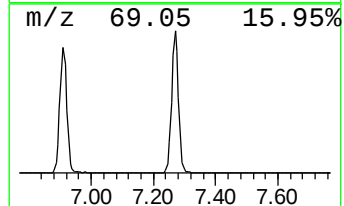
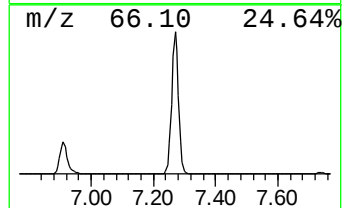
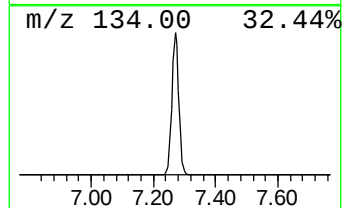
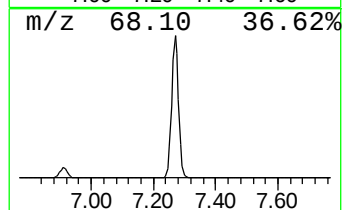
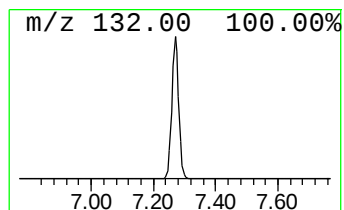
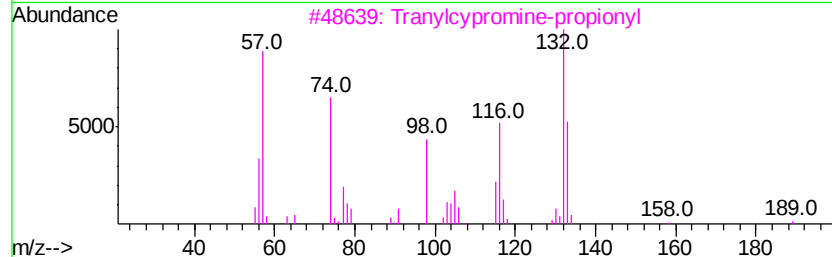
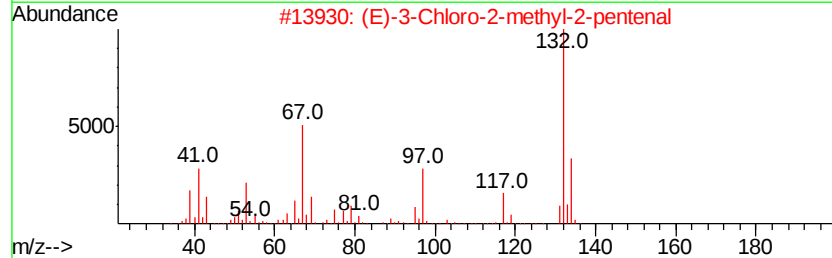
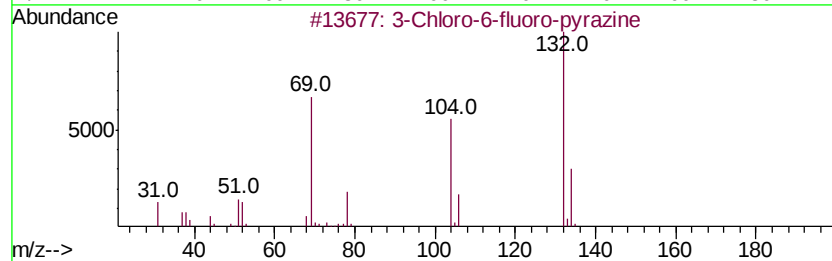
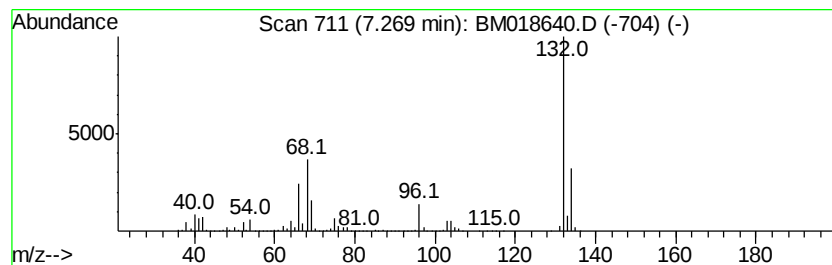
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	85.79 ng	6177570	1,4-Dichlorobenzene-d4	7.73

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	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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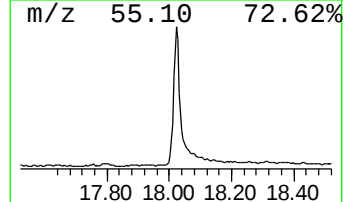
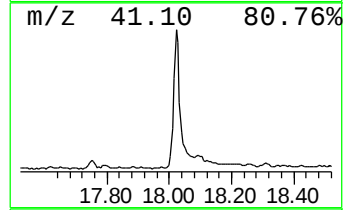
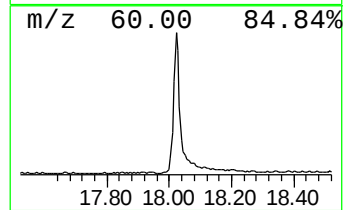
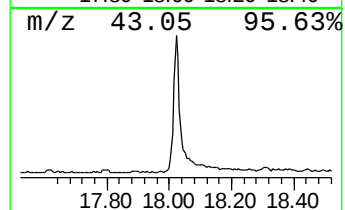
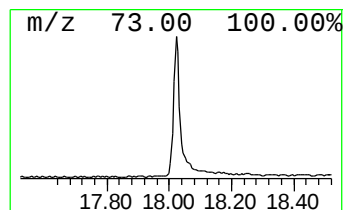
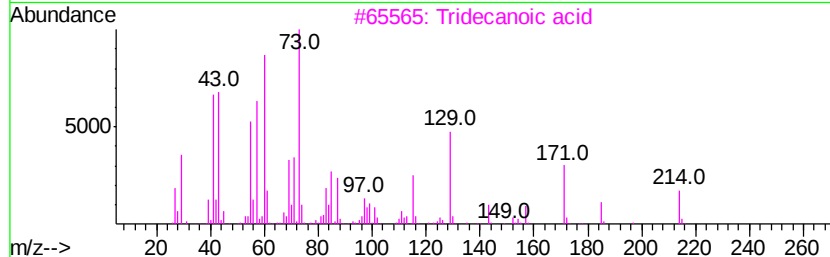
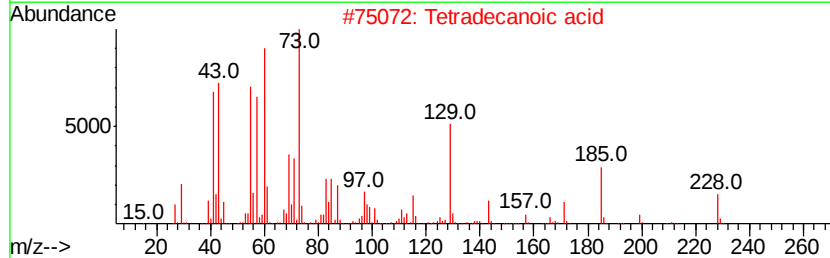
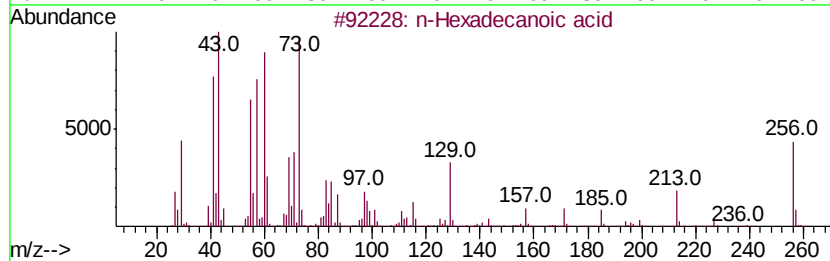
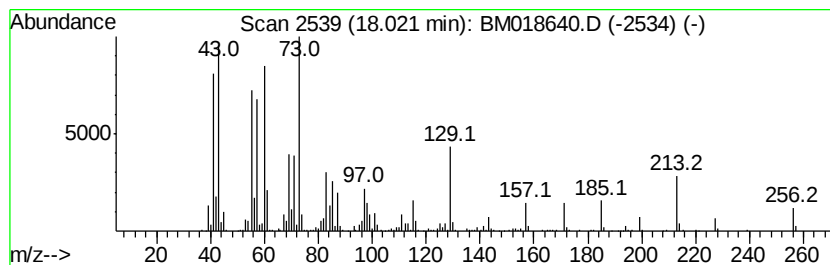
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.02	12.23 ng	1637060	Phenanthrene-d10	17.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	91
4		Undecanoic acid	186	C11H22O2	000112-37-8	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	76



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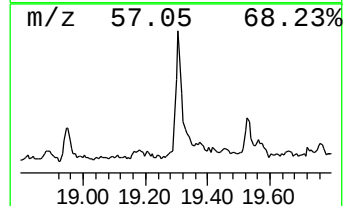
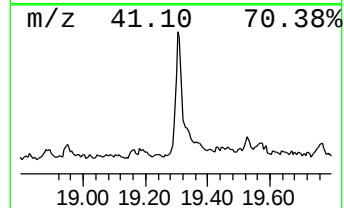
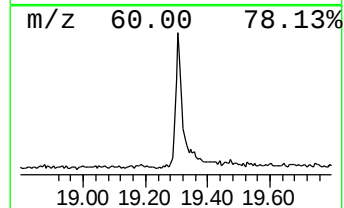
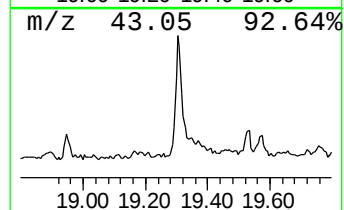
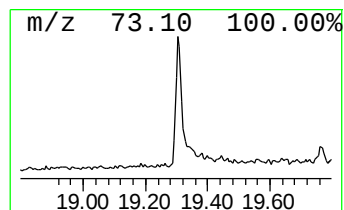
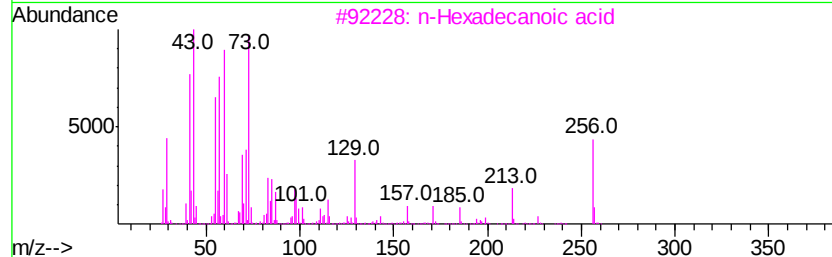
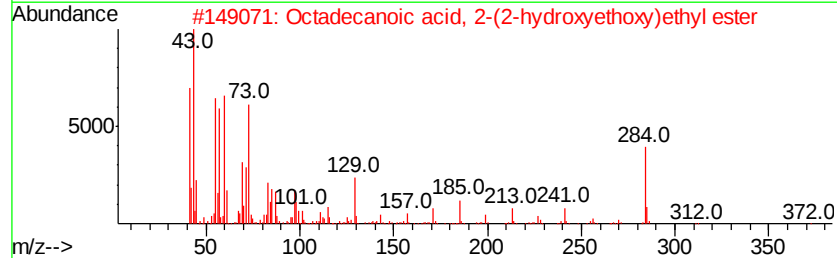
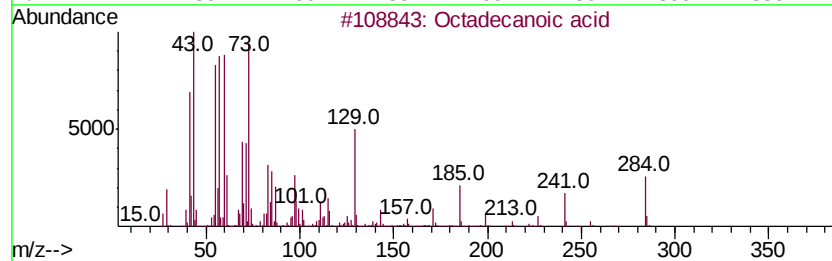
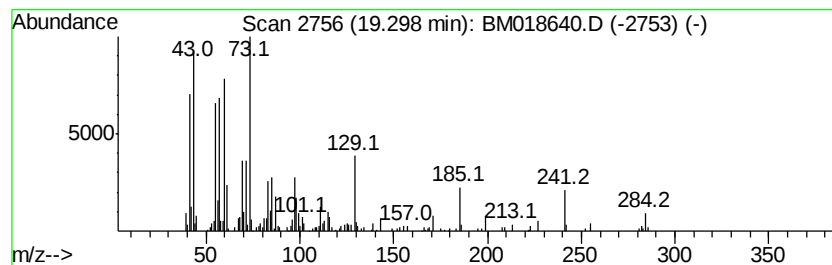
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 6 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.30	3.81 ng	628632	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	72



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Misc :
ALS Vial : 7 Sample Multiplier: 1

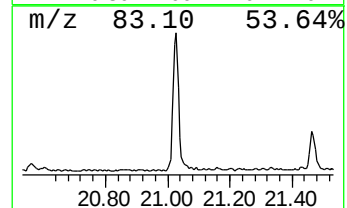
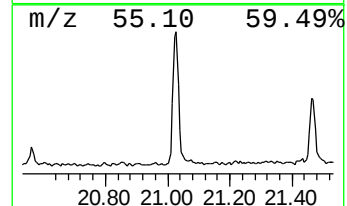
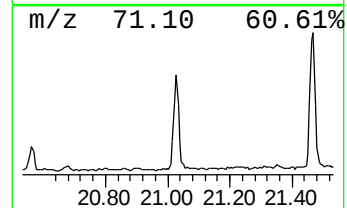
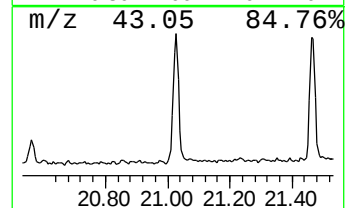
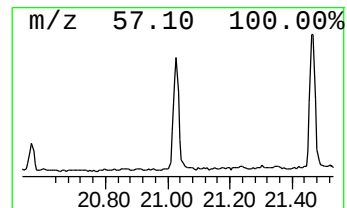
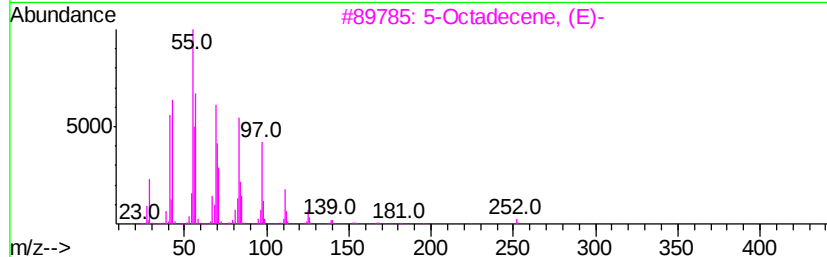
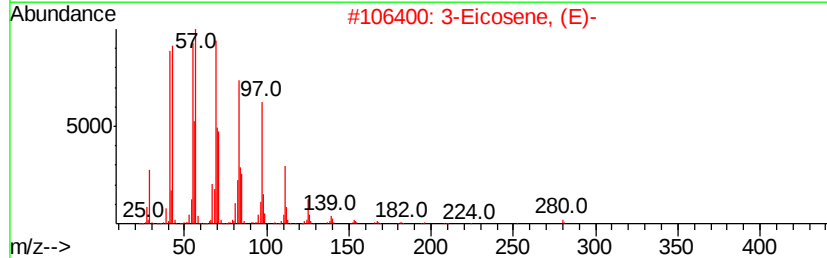
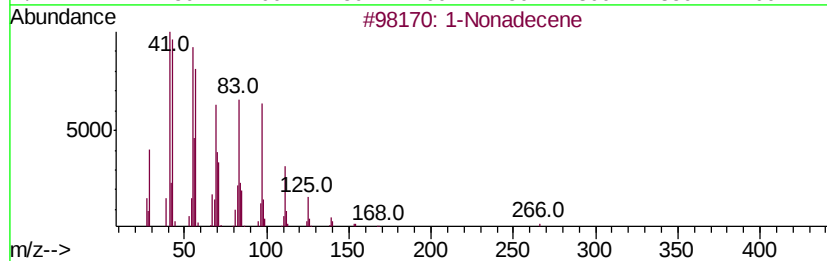
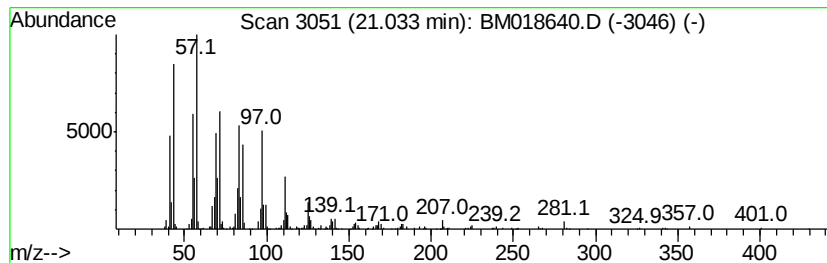
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	4.48 ng	738376	Chrysene-d12	21.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonadecene	266 C19H38	018435-45-5	98
2	3-Eicosene, (E)-	280 C20H40	074685-33-9	95
3	5-Octadecene, (E)-	252 C18H36	007206-21-5	91
4	Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1	90
5	1-Hexadecanesulfonyl chloride	324 C16H33ClO2S	038775-38-1	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
Data File : BM018640.D
Acq On : 18 Jan 2019 17:01
Operator : JU/SJ
Sample : K1173-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

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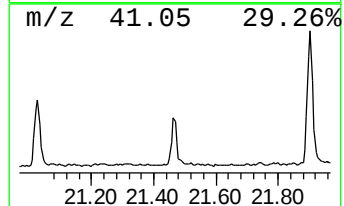
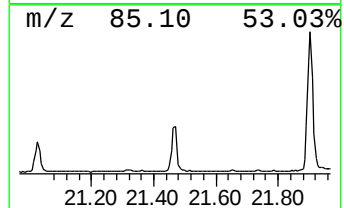
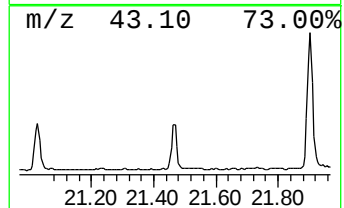
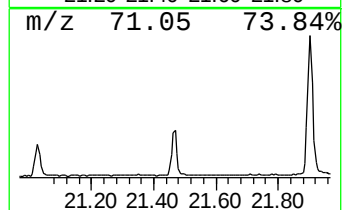
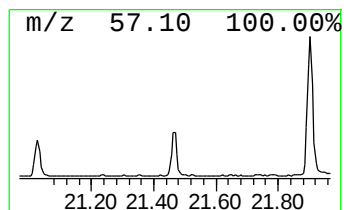
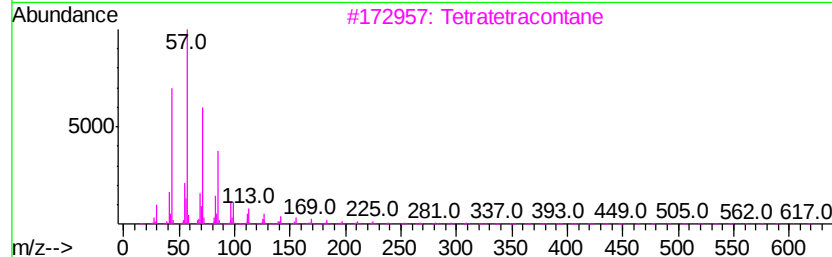
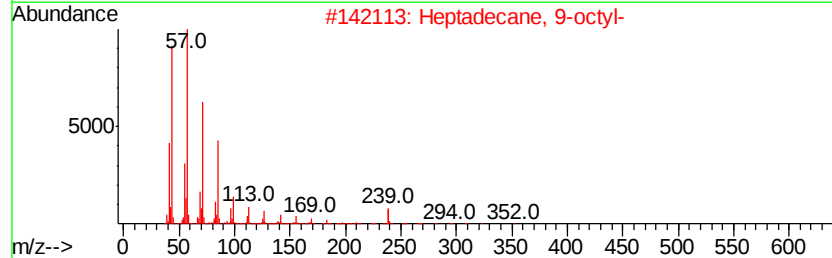
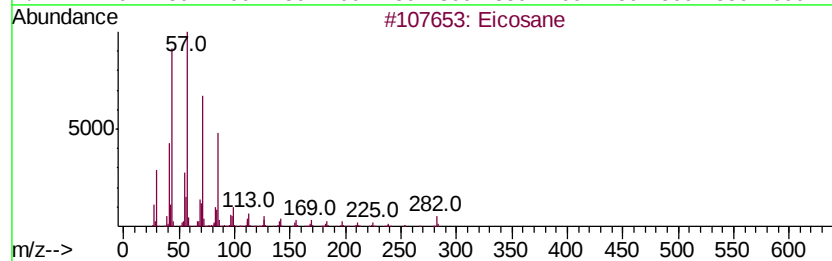
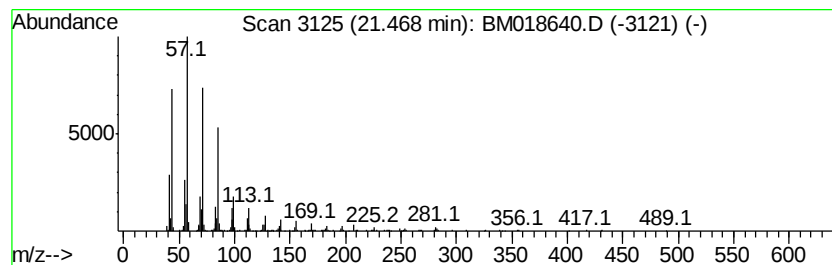
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	3.09 ng	509036	Chrysene-d12	21.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
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 Sample : K1173-03
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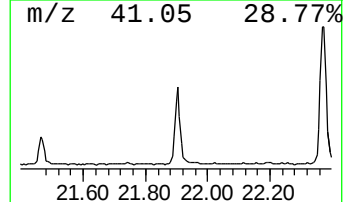
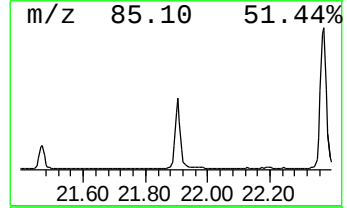
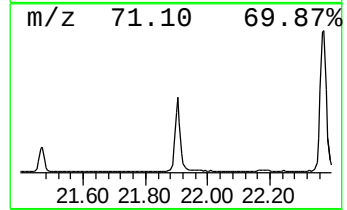
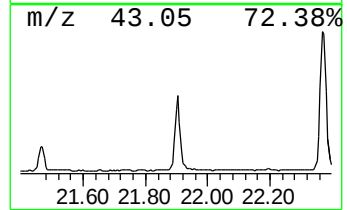
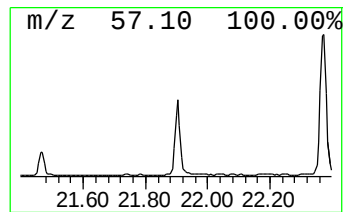
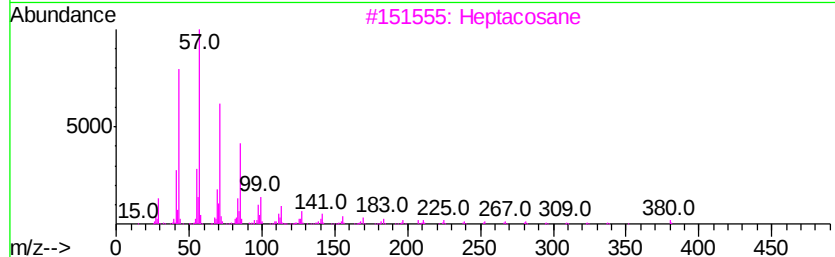
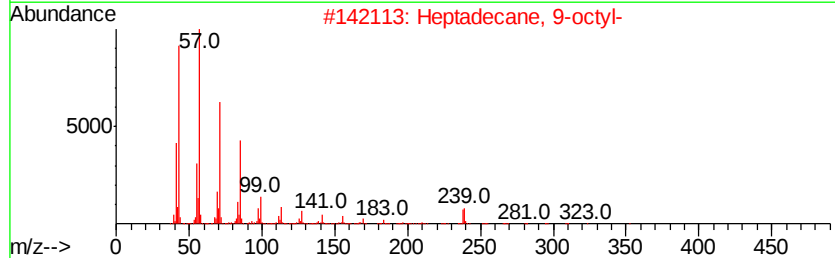
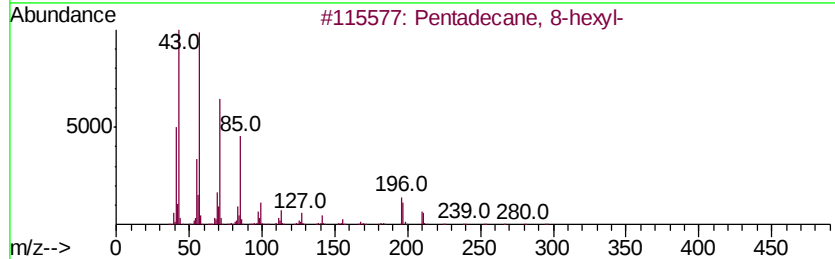
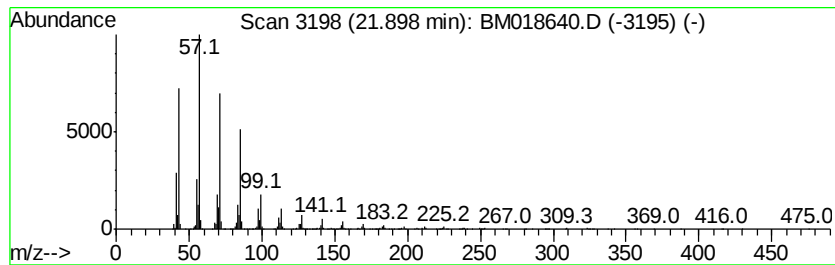
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
21.90	9.35 ng	1541420	Chrysene-d12		21.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Eicosane	282	C20H42	000112-95-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
Data File : BM018640.D
Acq On : 18 Jan 2019 17:01
Operator : JU/SJ
Sample : K1173-03
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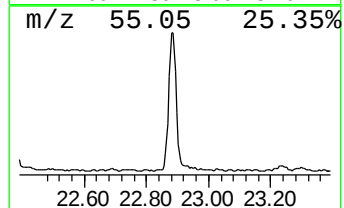
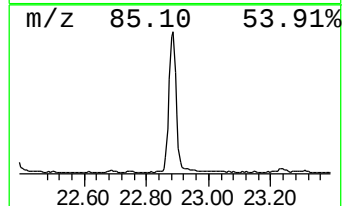
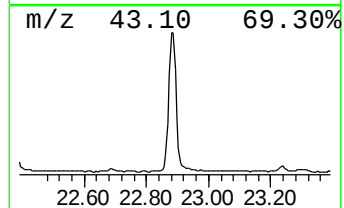
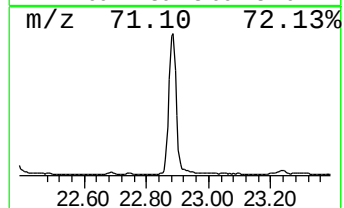
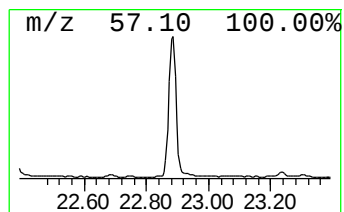
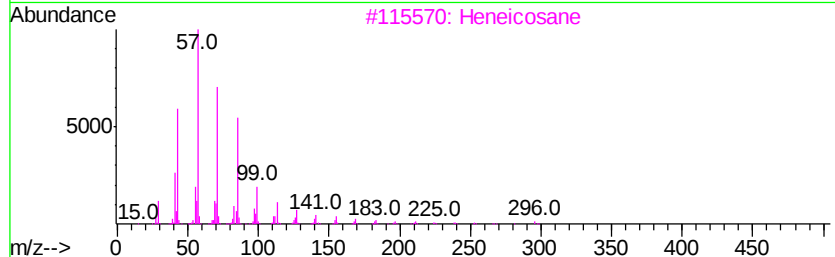
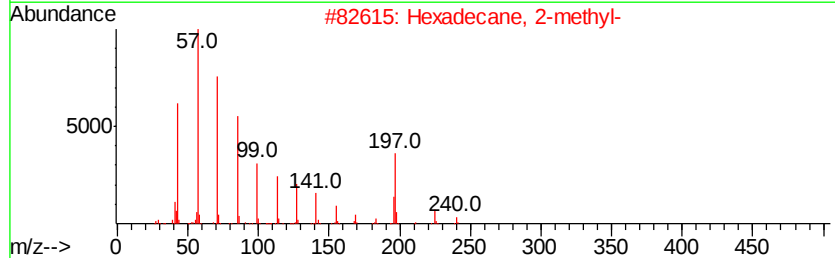
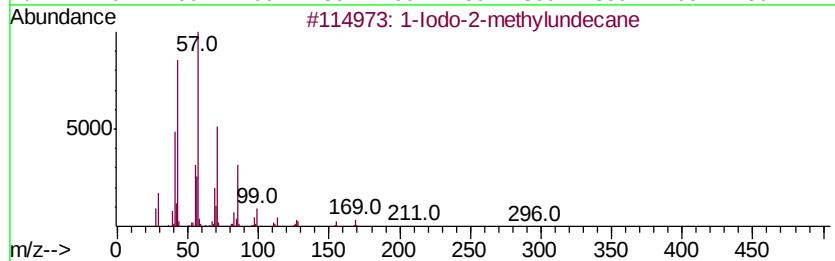
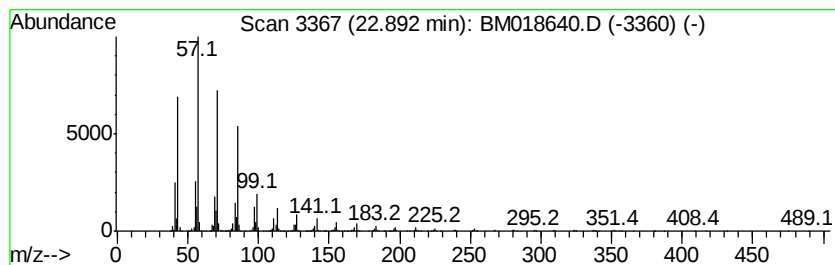
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Iodo-2-methylundecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.89	30.45 ng	4941980	Perylene-d12		23.60	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	93
2	Hexadecane, 2-methyl-		240	C17H36	001560-92-5	93
3	Heneicosane		296	C21H44	000629-94-7	91
4	Tetratriacontane		479	C34H70	014167-59-0	91
5	Tetratetracontane		619	C44H90	007098-22-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
Data File : BM018640.D
Acq On : 18 Jan 2019 17:01
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ALS Vial : 7 Sample Multiplier: 1

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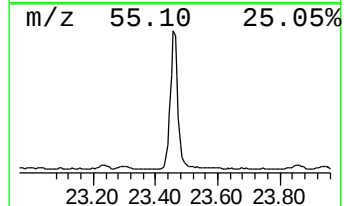
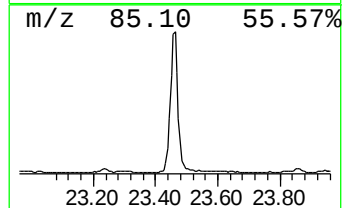
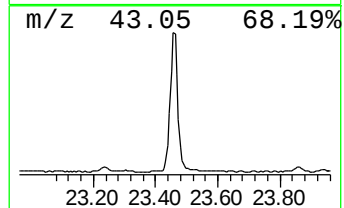
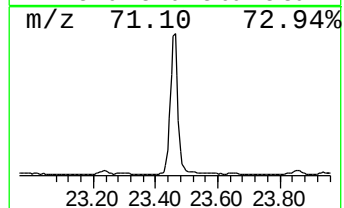
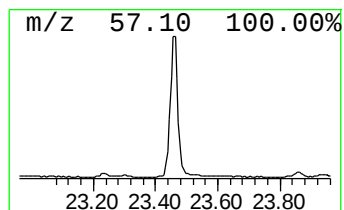
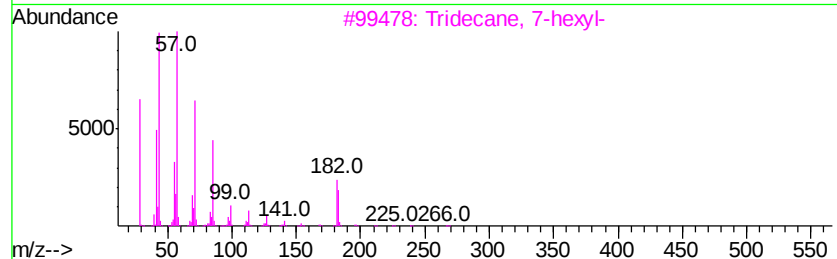
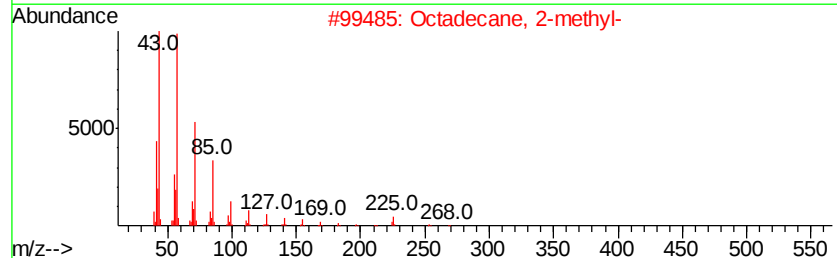
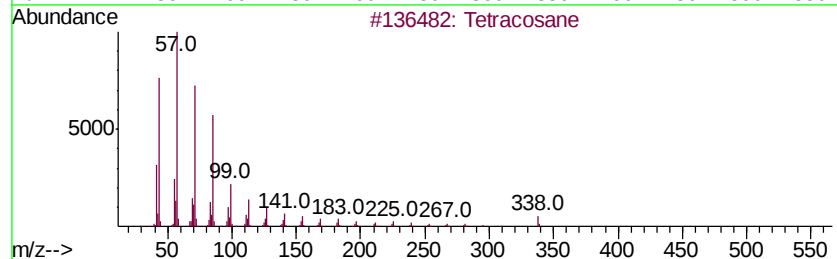
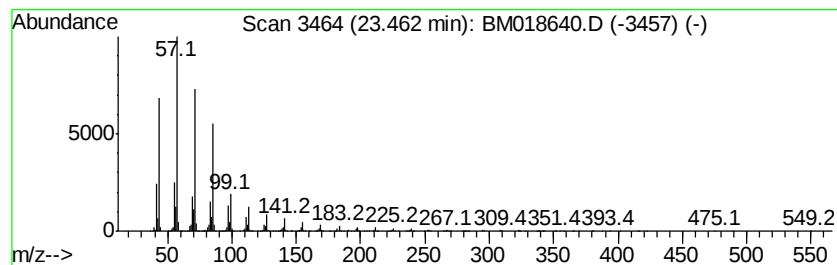
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.46	33.83 ng	5490120	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	98
2		Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
3		Tridecane, 7-hexyl-	268	C19H40	007225-66-3	93
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Tetratriacontane	479	C34H70	014167-59-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
Data File : BM018640.D
Acq On : 18 Jan 2019 17:01
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Misc :
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Instrument :
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ClientSampleId :
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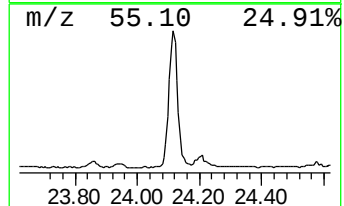
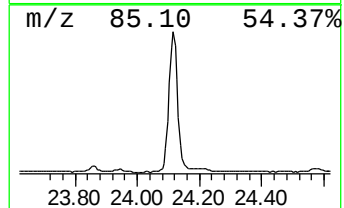
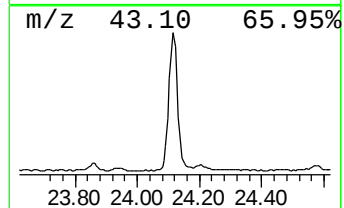
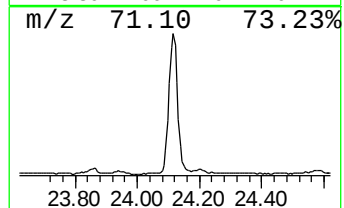
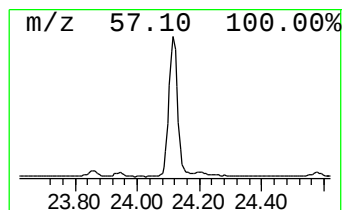
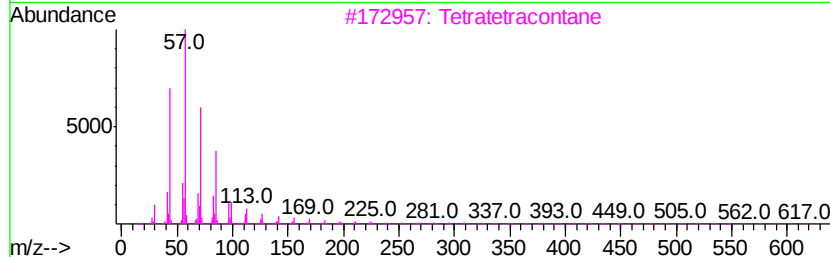
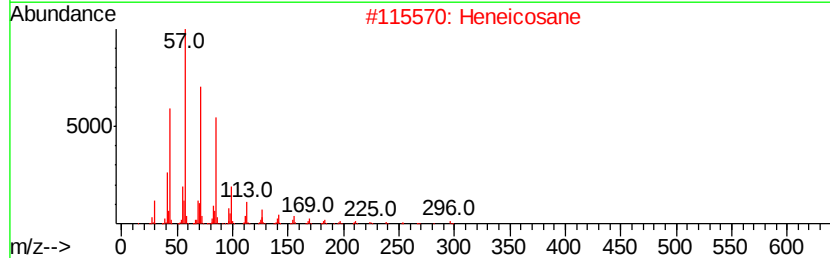
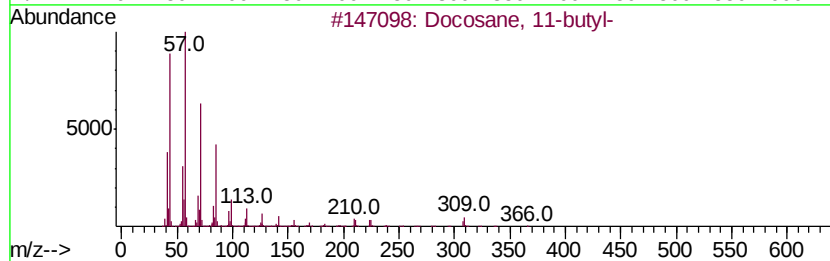
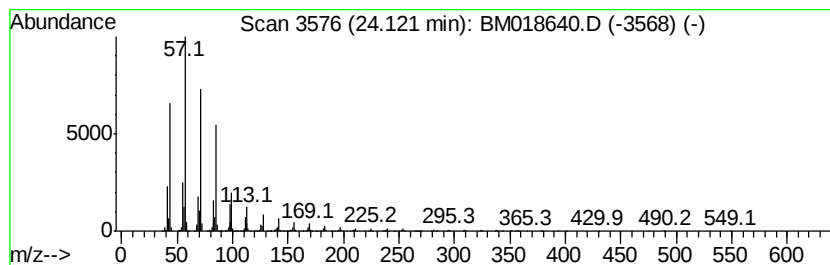
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Docosane, 11-butyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.12	28.29 ng	4591900	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		Docosane, 9-butyl-	366	C26H54	055282-14-9	91
5		Tetratriacontane	479	C34H70	014167-59-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
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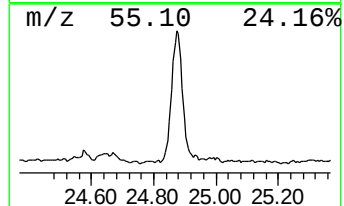
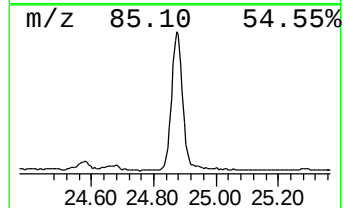
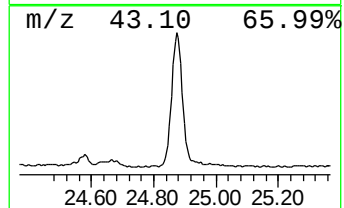
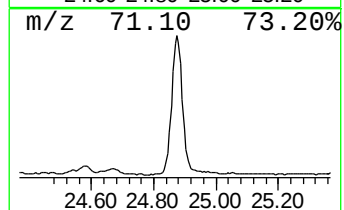
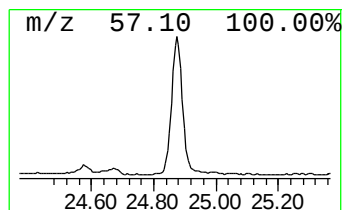
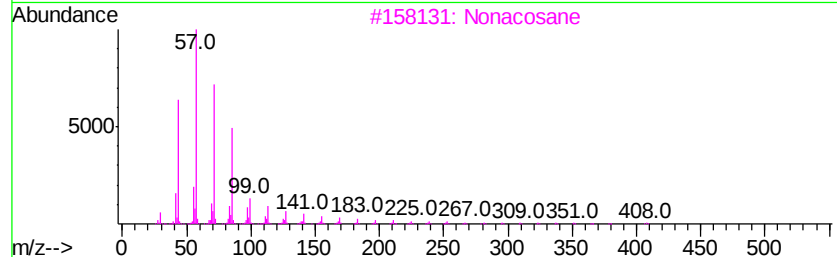
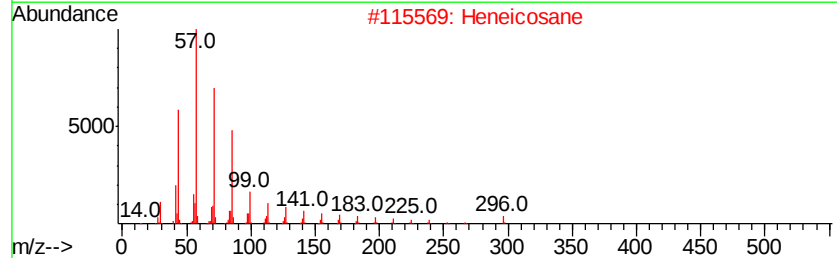
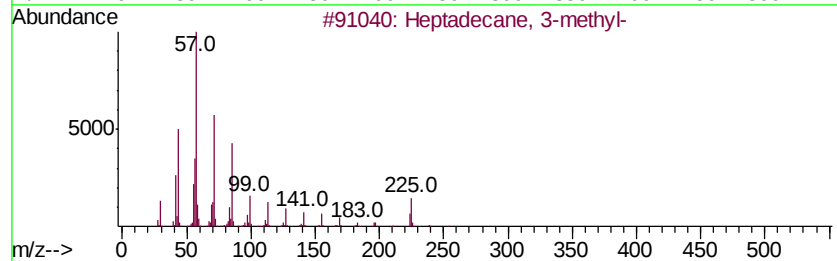
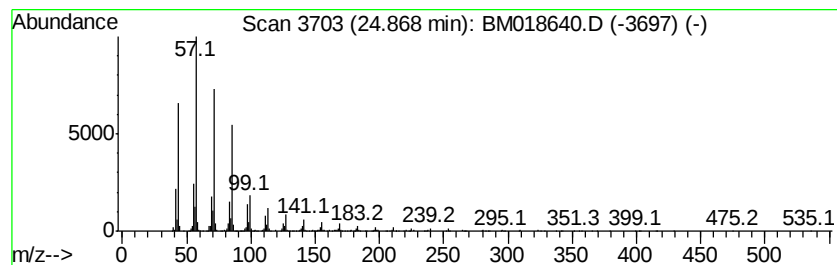
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heptadecane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.87	15.22 ng	2469640	Perylene-d12	23.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	93
2		Heneicosane	296	C21H44	000629-94-7	91
3		Nonacosane	408	C29H60	000630-03-5	91
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM011819\
Data File : BM018640.D
Acq On : 18 Jan 2019 17:01
Operator : JU/SJ
Sample : K1173-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200050

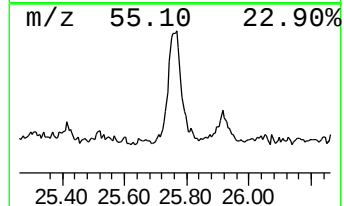
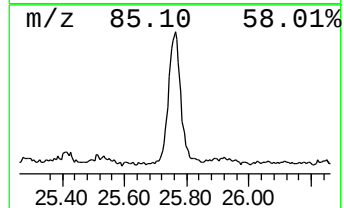
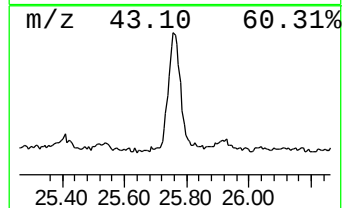
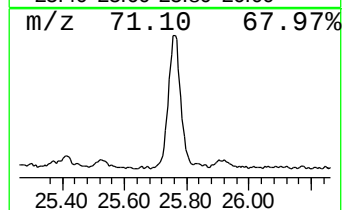
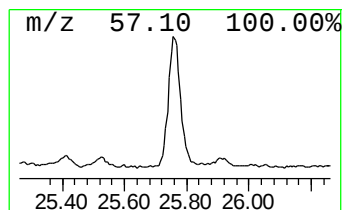
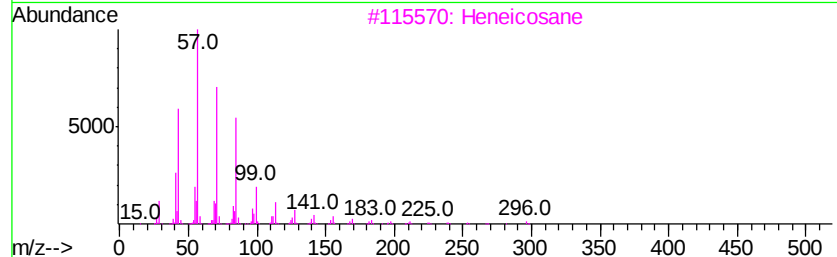
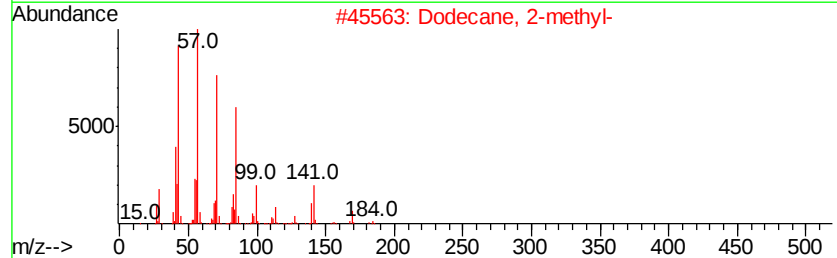
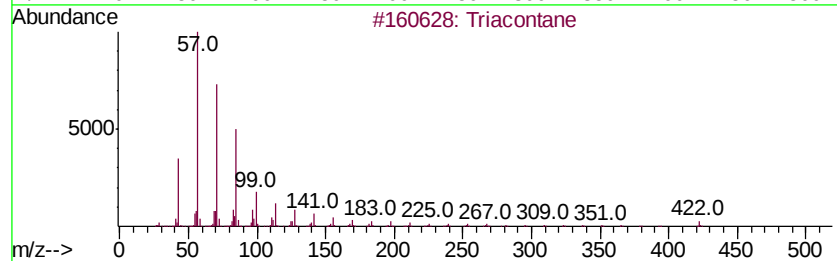
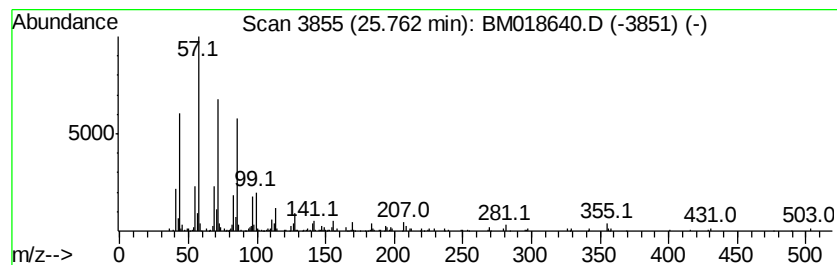
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Triacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.76	4.38 ng	710388	Perylene-d12	23.60

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	87
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM011819\
Data File : BM018640.D
Acq On : 18 Jan 2019 17:01
Operator : JU/SJ
Sample : K1173-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
RBR-200050

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM010919.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
R-(-)-1,2-propane...	3.52	3.9	ng	278388	1	7.73	1440160	20.0
unknown4.88	4.88	3.9	ng	282132	1	7.73	1440160	20.0
unknown7.27	7.27	85.8	ng	6177570	1	7.73	1440160	20.0
n-Hexadecanoic acid	18.02	12.2	ng	1637060	4	17.13	2677450	20.0
Octadecanoic acid	19.30	3.8	ng	628632	5	21.33	3298020	20.0
1-Nonadecene	21.03	4.5	ng	738376	5	21.33	3298020	20.0
Eicosane	21.47	3.1	ng	509036	5	21.33	3298020	20.0
Pentadecane, 8-he...	21.90	9.3	ng	1541420	5	21.33	3298020	20.0
1-Iodo-2-methylun...	22.89	30.4	ng	4941980	6	23.60	3246100	20.0
Tetracosane	23.46	33.8	ng	5490120	6	23.60	3246100	20.0
Docosane, 11-butyl-	24.12	28.3	ng	4591900	6	23.60	3246100	20.0
Heptadecane, 3-me...	24.87	15.2	ng	2469640	6	23.60	3246100	20.0
Triacontane	25.76	4.4	ng	710388	6	23.60	3246100	20.0