

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
 Data File : BM018473.D
 Acq On : 09 Jan 2019 15:15
 Operator : JU/SJ
 Sample : K1088-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CPSB-07(15-20)

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	4.298	202	206	212	rBV	225555	296276	1.01%	0.115%
2	4.898	303	308	316	rVB	254841	362834	1.24%	0.140%
3	5.351	378	385	402	rVB	5605998	7963979	27.13%	3.079%
4	6.934	646	654	669	rBV	5167545	8710130	29.67%	3.367%
5	7.298	708	716	725	rBV	5665671	9087350	30.95%	3.513%
6	7.763	788	795	802	rBV	1688248	2676296	9.12%	1.035%
7	8.081	841	849	855	rBV	4081574	6547451	22.30%	2.531%
8	8.928	985	993	1001	rBV	3114615	5125961	17.46%	1.982%
9	10.551	1262	1269	1276	rBV	2186466	3573089	12.17%	1.381%
10	13.027	1682	1690	1697	rBV	7599915	11109635	37.84%	4.295%
11	13.745	1804	1812	1817	rBV	187051	330560	1.13%	0.128%
12	13.868	1827	1833	1839	rBV	904313	1300043	4.43%	0.503%
13	14.410	1919	1925	1931	rVV2	3124688	4682616	15.95%	1.810%
14	14.468	1931	1935	1942	rVB	243927	403541	1.37%	0.156%
15	15.904	2173	2179	2185	rBV	6336340	9102072	31.00%	3.519%
16	16.127	2210	2217	2224	rBV3	387428	681454	2.32%	0.263%
17	16.951	2353	2357	2363	rVB	576306	827516	2.82%	0.320%
18	17.156	2387	2392	2397	rBV	4007695	5726643	19.51%	2.214%
19	17.556	2457	2460	2467	rBV	212905	344795	1.17%	0.133%
20	18.068	2539	2547	2562	rBV	16039602	29356846	100.00%	11.349%
21	18.968	2698	2700	2703	rBV2	268217	304893	1.04%	0.118%
22	19.003	2703	2706	2710	rVB3	494084	611753	2.08%	0.236%
23	19.162	2721	2733	2740	rBV	6375820	21844281	74.41%	8.445%
24	19.345	2758	2764	2781	rBV	18154663	28962896	98.66%	11.197%
25	19.792	2835	2840	2848	rVB	13358499	15950026	54.33%	6.166%
26	20.668	2978	2989	2998	rVB	9365429	26620171	90.68%	10.291%
27	21.056	3052	3055	3063	rVB	1839624	2315281	7.89%	0.895%
28	21.350	3101	3105	3110	rVB	5027458	6357664	21.66%	2.458%
29	21.644	3147	3155	3161	rVV	10878159	22661557	77.19%	8.761%
30	21.715	3163	3167	3182	rVB2	2212077	5007140	17.06%	1.936%
31	22.568	3305	3312	3323	rVB	5663000	15695883	53.47%	6.068%
32	23.609	3483	3489	3490	rBV	2466653	4129389	14.07%	1.596%

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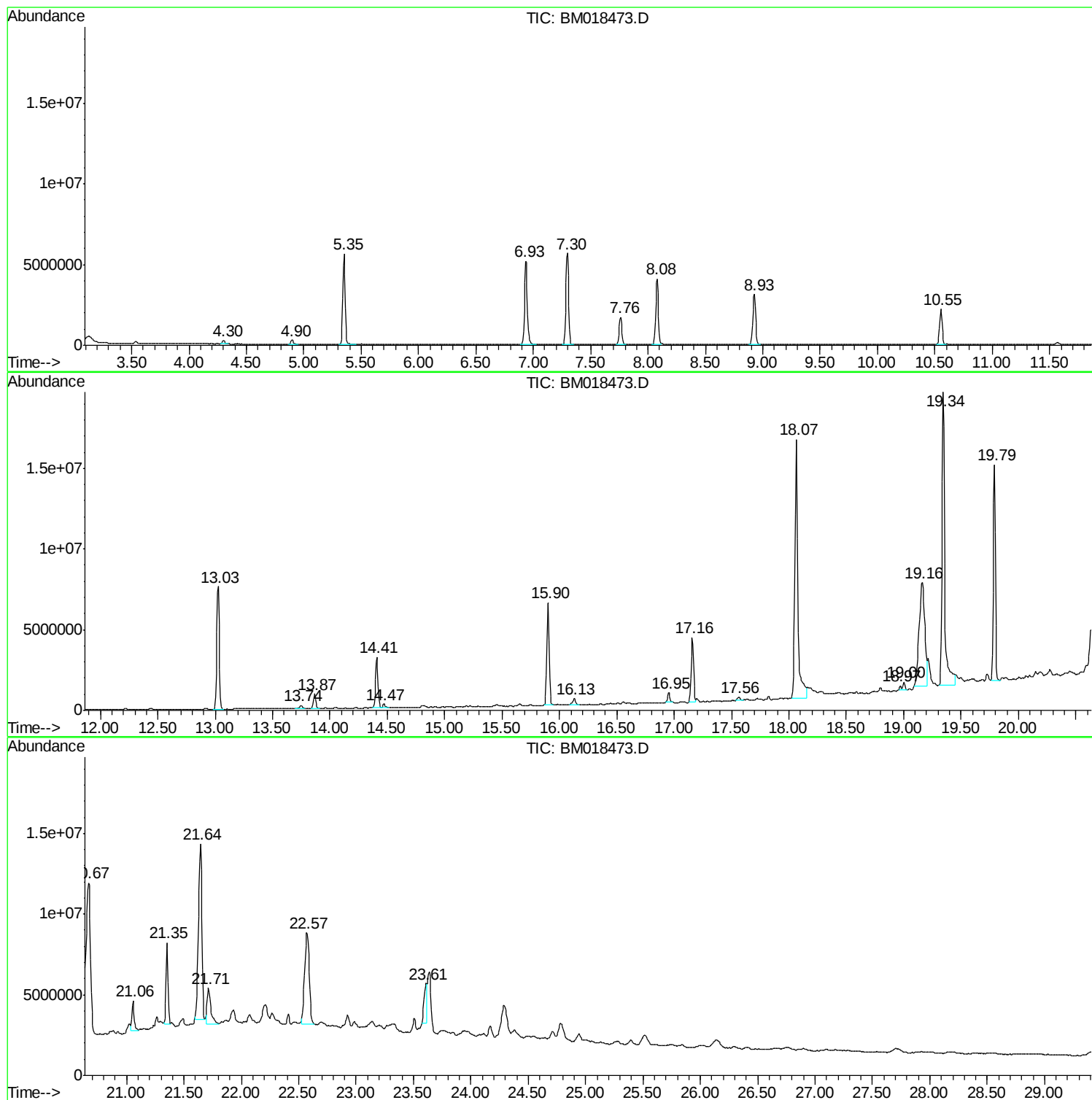
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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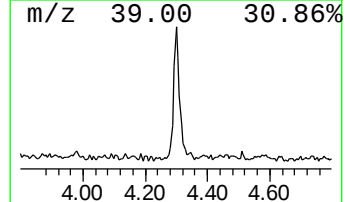
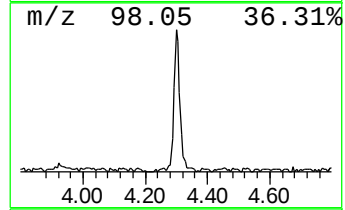
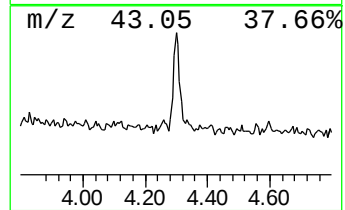
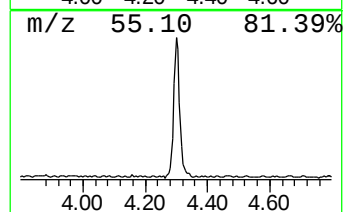
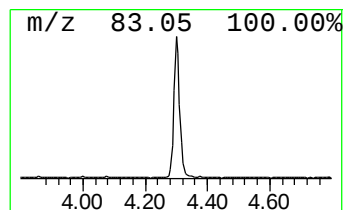
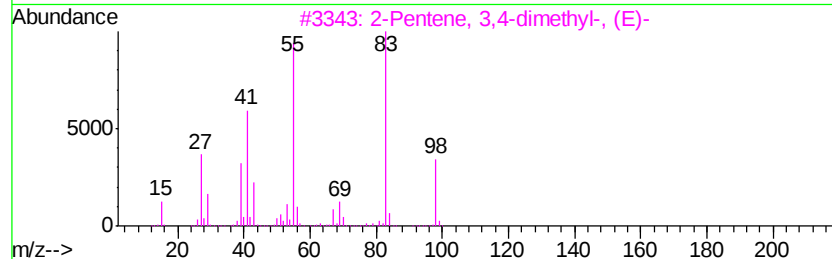
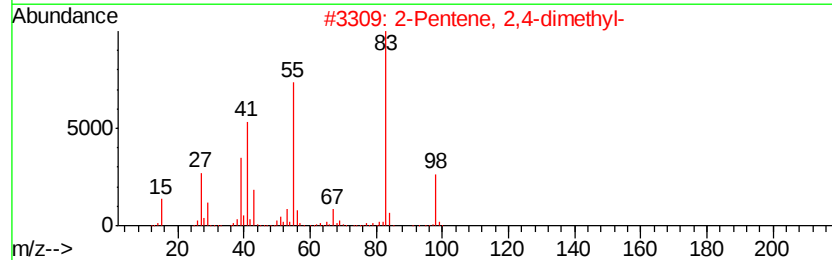
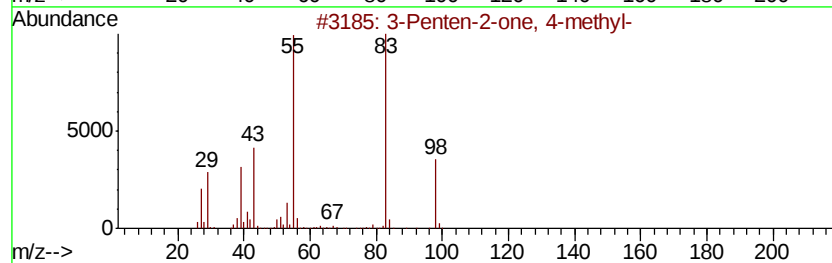
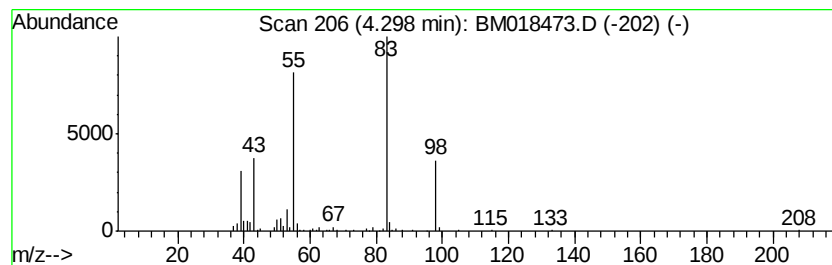
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	2.21 ng	296276	1,4-Dichlorobenzene-d4	7.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	93
2			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			3-Hexen-2-one	98	C6H10O	000763-93-9	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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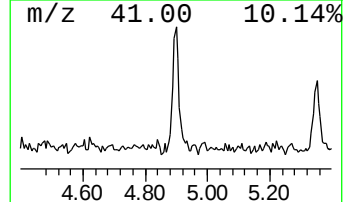
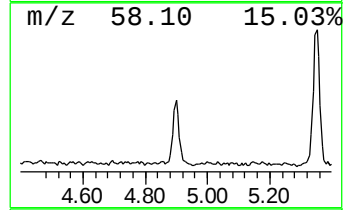
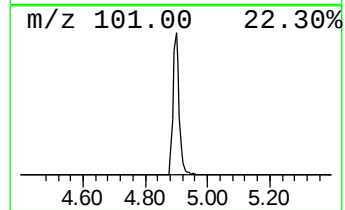
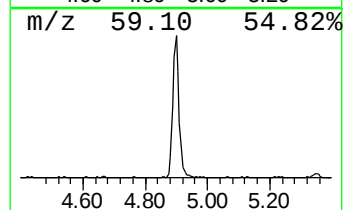
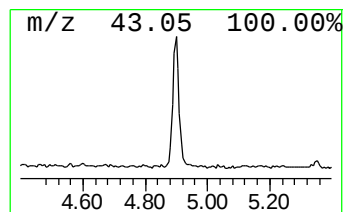
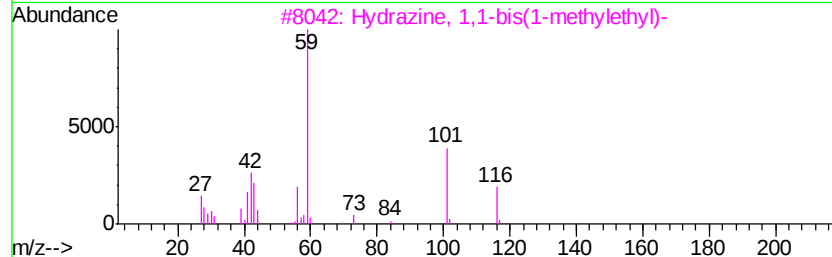
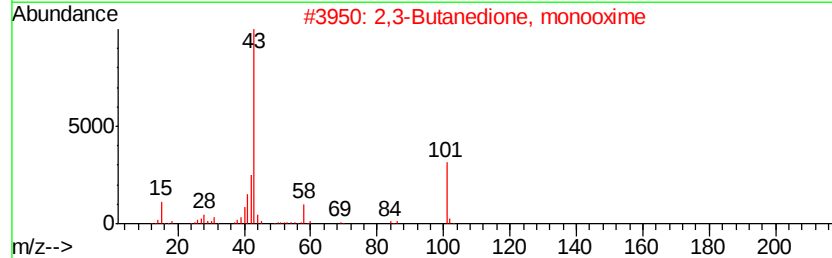
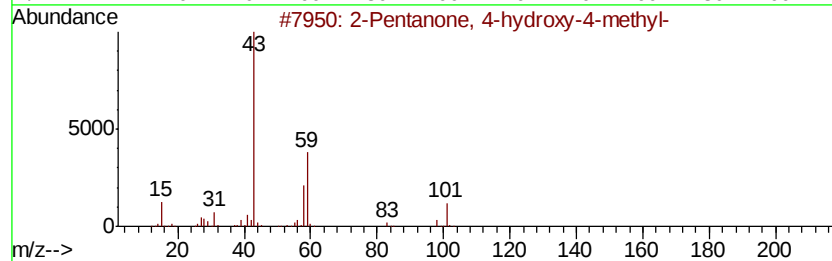
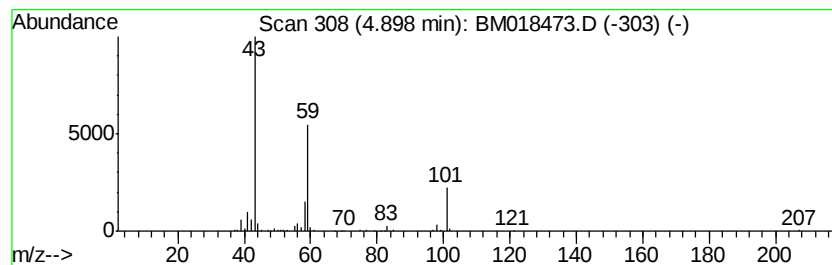
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.71 ng	362834	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	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
4		Propanoic acid, 3-nitro-, methyl...	133	C4H7NO4	020497-95-4	17
5		4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	12



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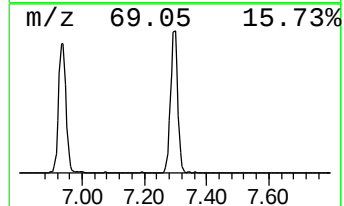
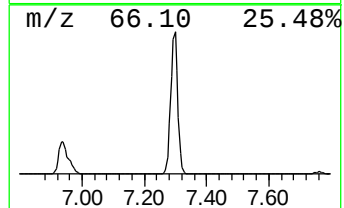
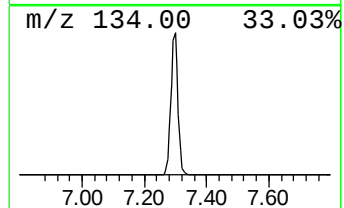
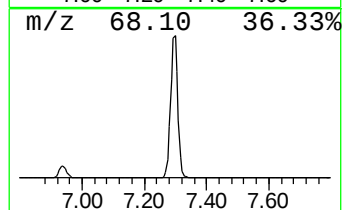
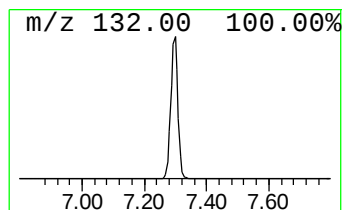
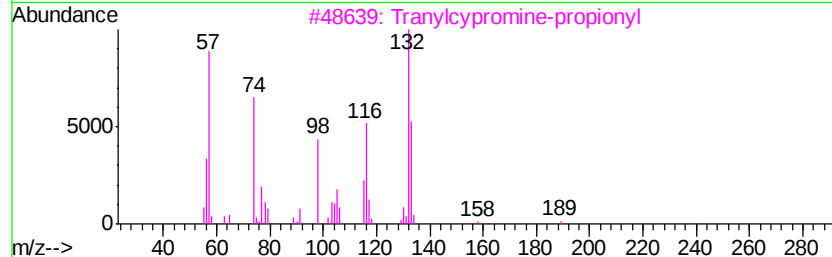
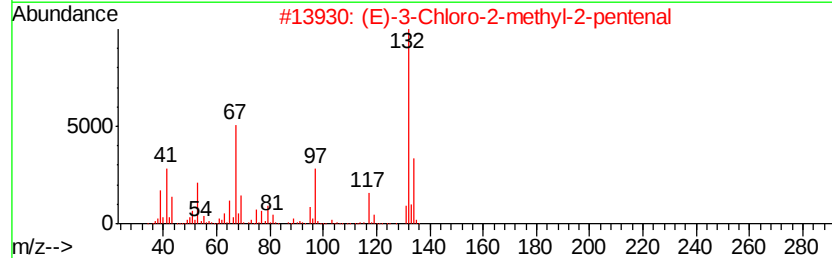
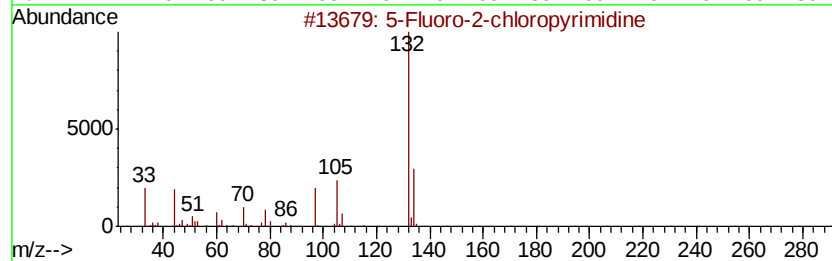
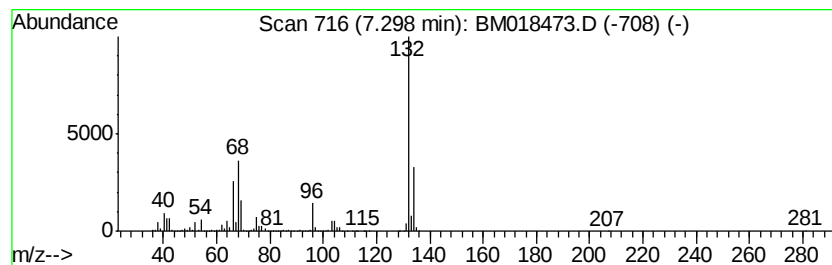
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.30 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	67.91 ng	9087350	1,4-Dichlorobenzene-d4	7.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	16
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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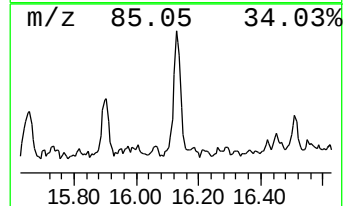
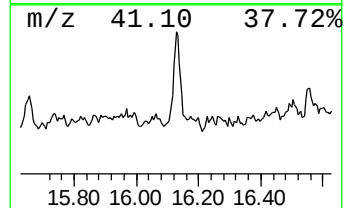
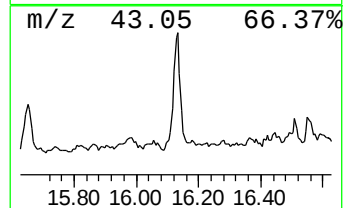
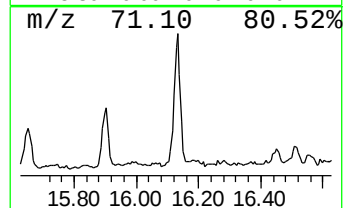
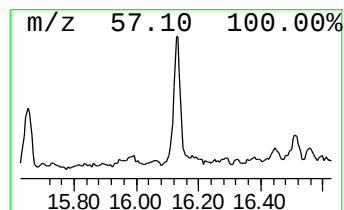
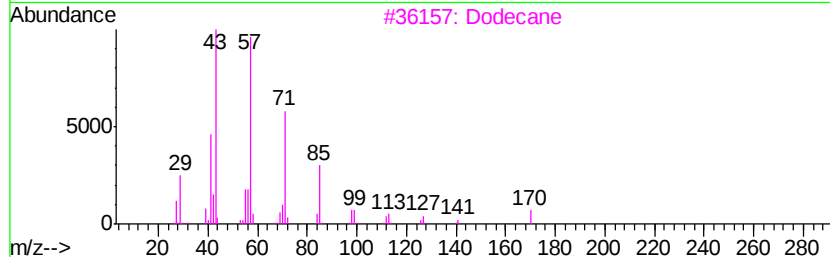
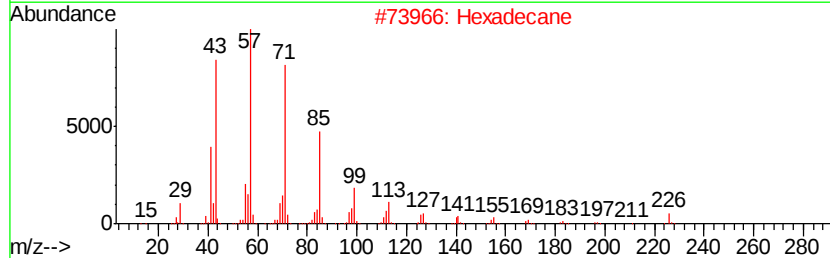
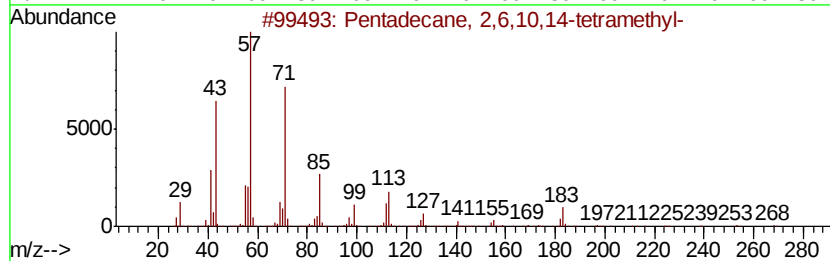
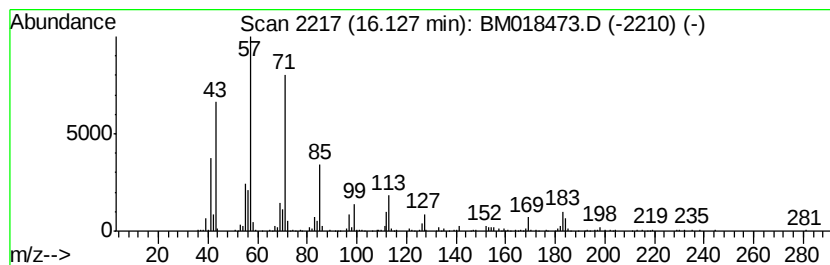
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.38 ng	681454	Phenanthrene-d10	17.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	86
2		Hexadecane	226	C16H34	000544-76-3	74
3		Dodecane	170	C12H26	000112-40-3	74
4		Undecane, 2-methyl-	170	C12H26	007045-71-8	64
5		Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	64



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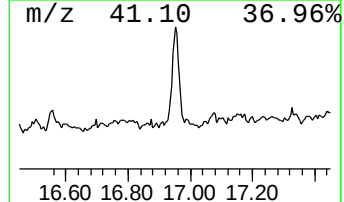
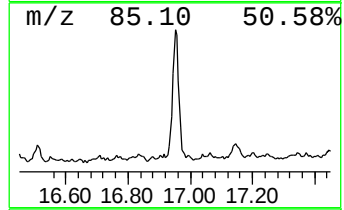
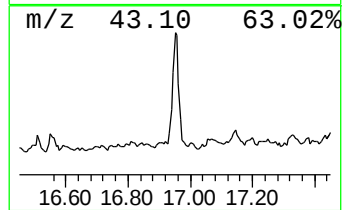
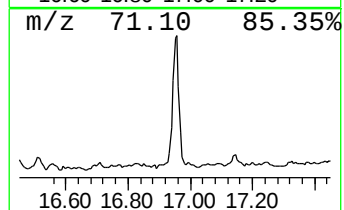
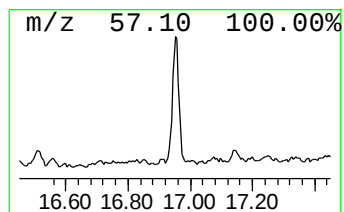
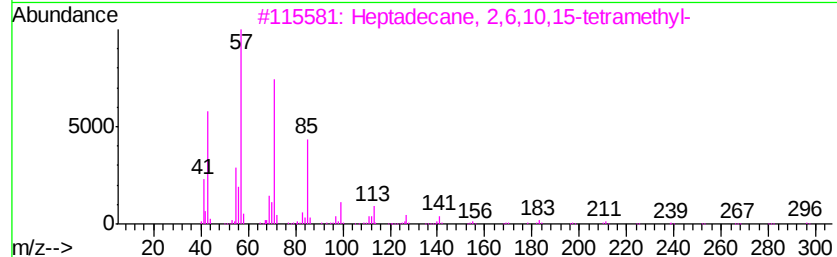
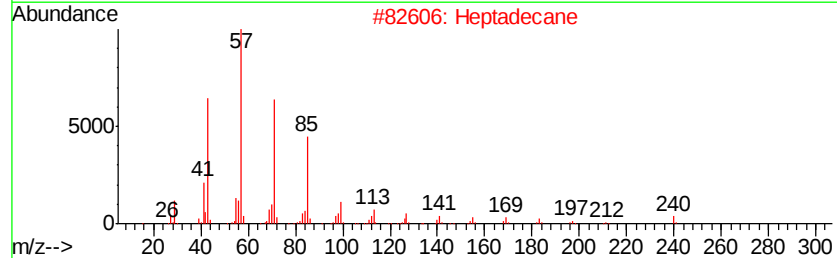
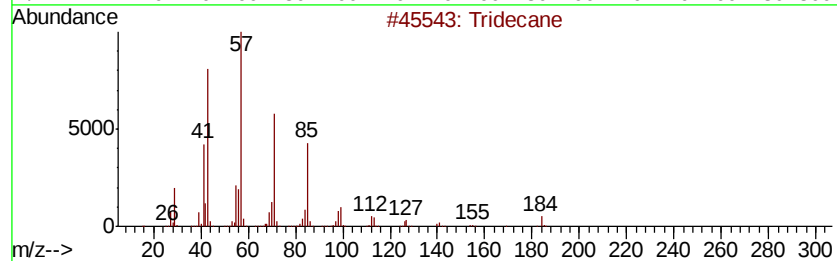
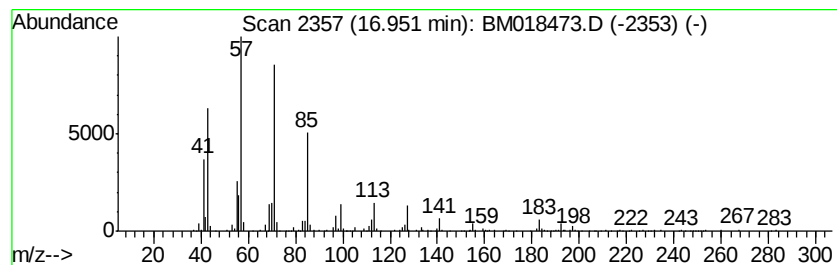
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tridecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.95	2.89 ng	827516	Phenanthrene-d10	17.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tridecane	184	C13H28	000629-50-5	87
2		Heptadecane	240	C17H36	000629-78-7	86
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86
4		Pentadecane, 4-methyl-	226	C16H34	002801-87-8	86
5		Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
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 Operator : JU/SJ
 Sample : K1088-01
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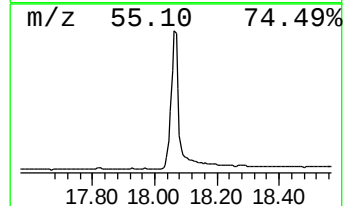
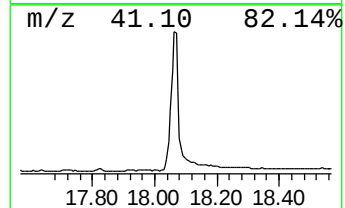
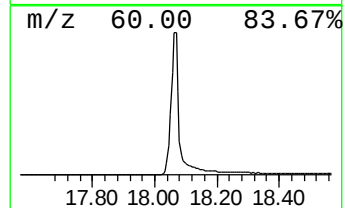
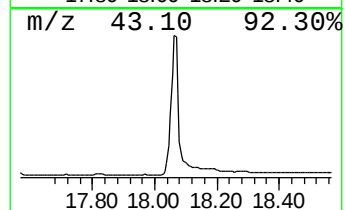
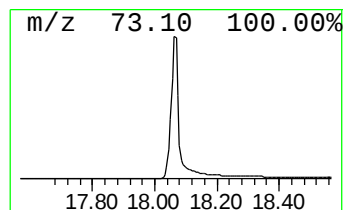
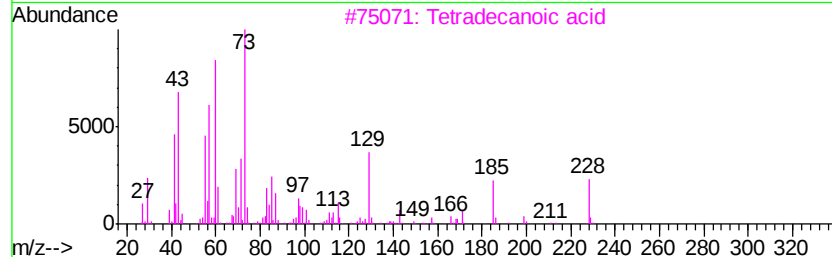
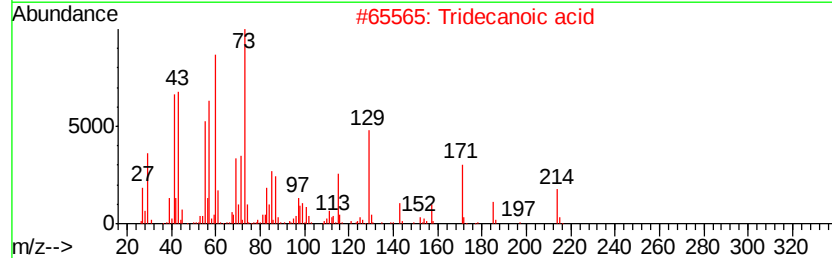
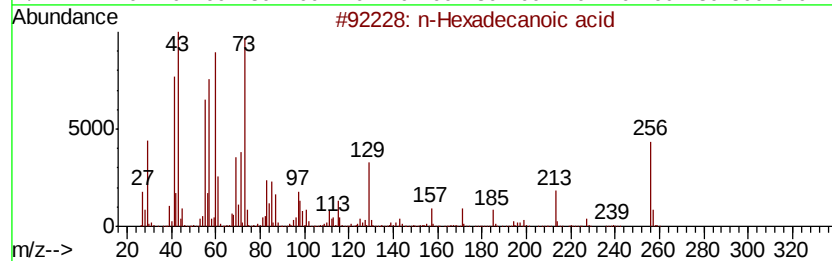
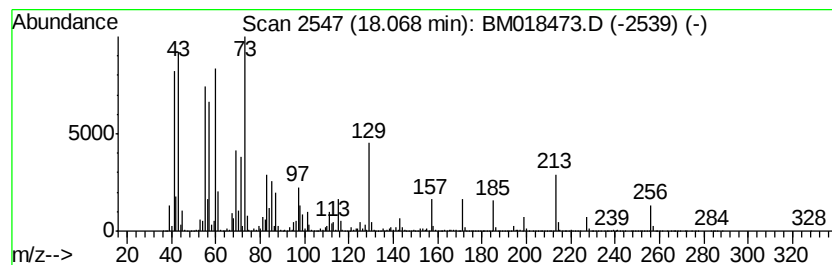
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.		
18.07	102.53 ng	29356800	Phenanthrene-d10		17.16		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018473.D
Acq On : 09 Jan 2019 15:15
Operator : JU/SJ
Sample : K1088-01
Misc :
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Instrument :
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ClientSampleId :
CPSB-07(15-20)

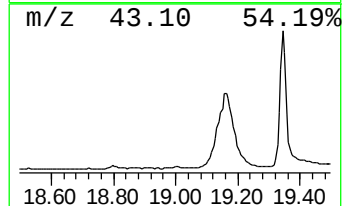
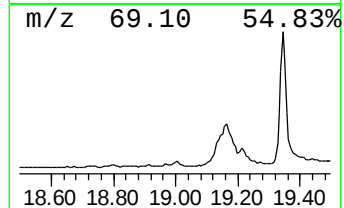
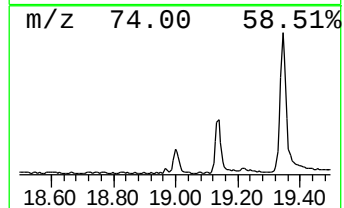
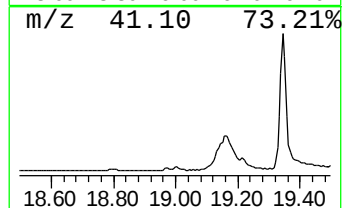
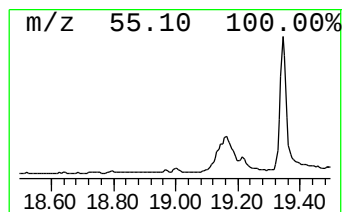
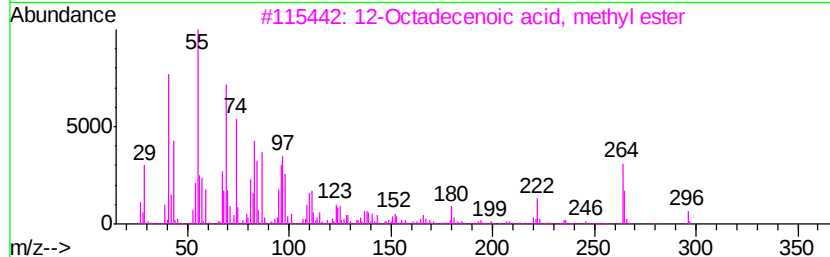
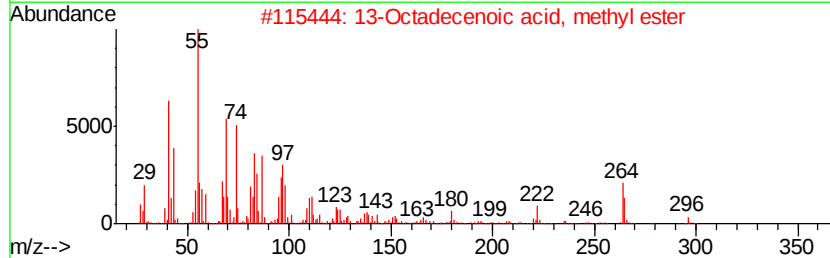
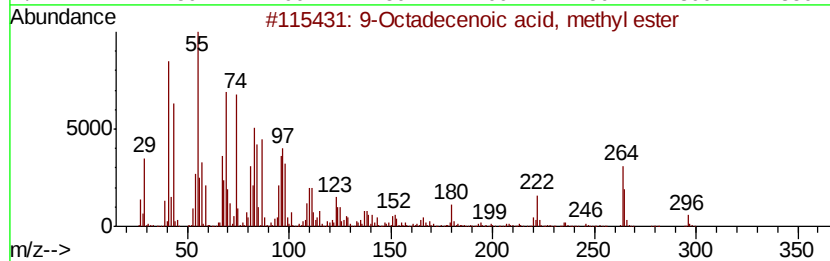
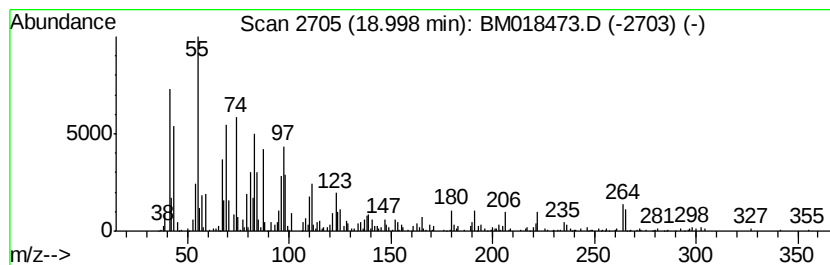
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenoic acid, methyl... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.00	2.14 ng	611753	Phenanthrene-d10	17.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	91
2		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91
3		12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	87
4		10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87
5		9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018473.D
Acq On : 09 Jan 2019 15:15
Operator : JU/SJ
Sample : K1088-01
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ClientSampleId :
CPSB-07(15-20)

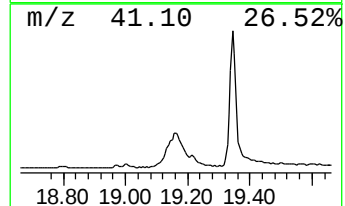
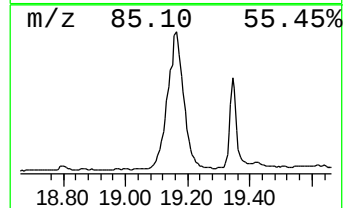
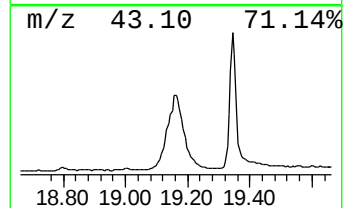
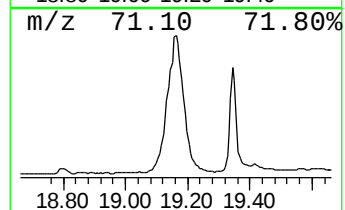
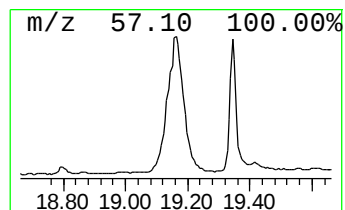
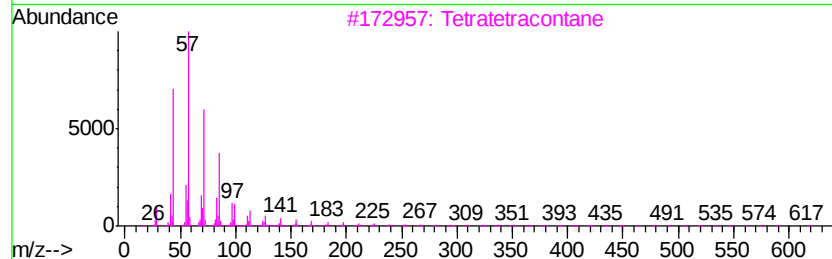
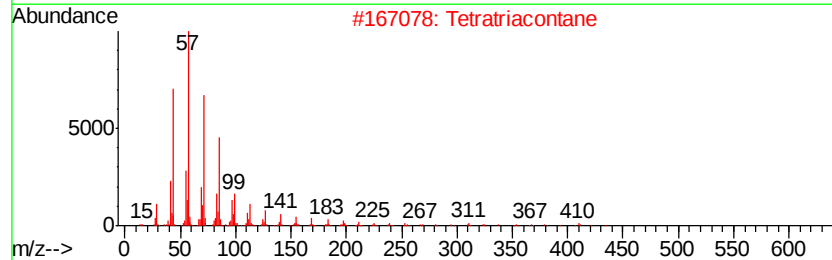
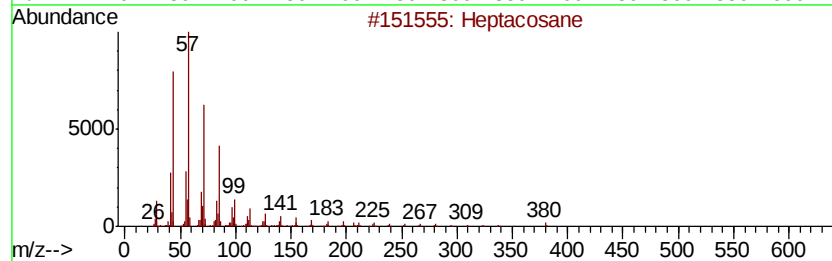
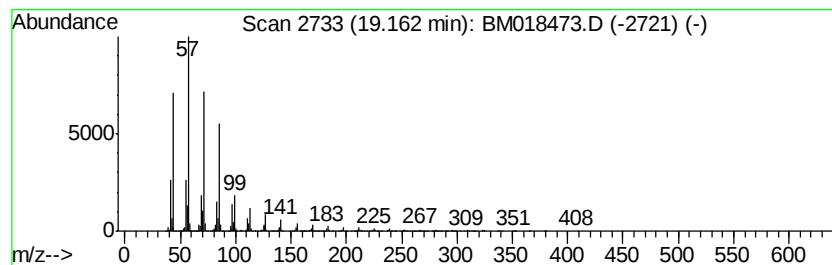
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.16	76.29 ng	21844300	Phenanthrene-d10	17.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Tetratriacontane		479	C34H70	014167-59-0	91
3	Tetratetracontane		619	C44H90	007098-22-8	91
4	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
5	Heneicosane		296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018473.D
Acq On : 09 Jan 2019 15:15
Operator : JU/SJ
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Instrument :
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ClientSampleId :
CPSB-07(15-20)

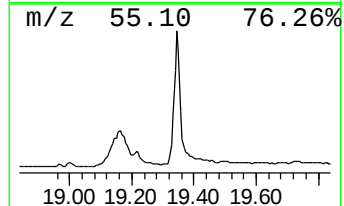
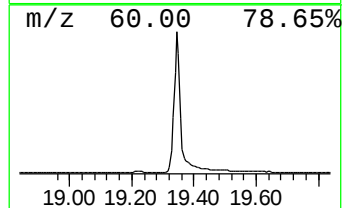
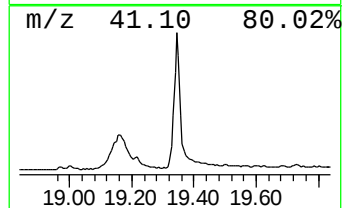
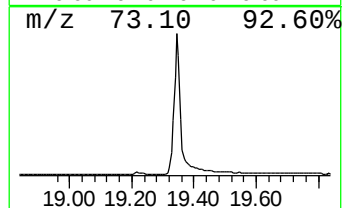
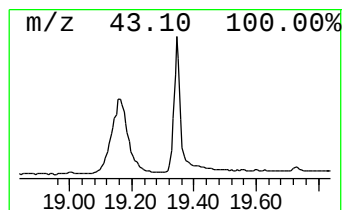
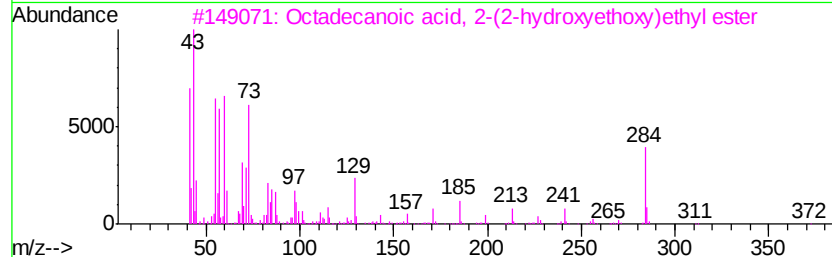
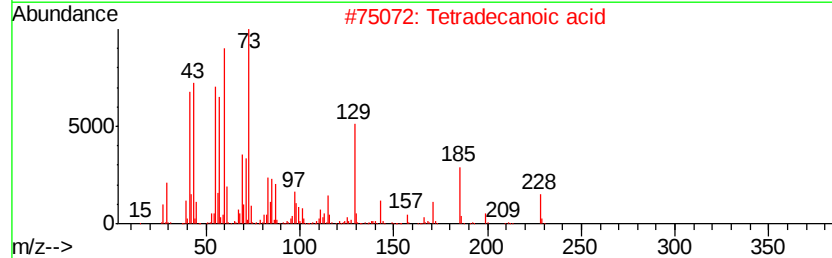
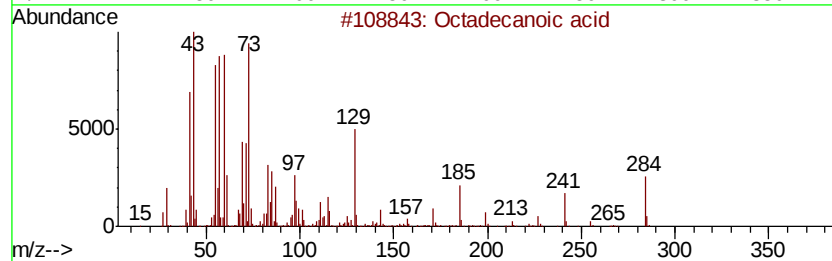
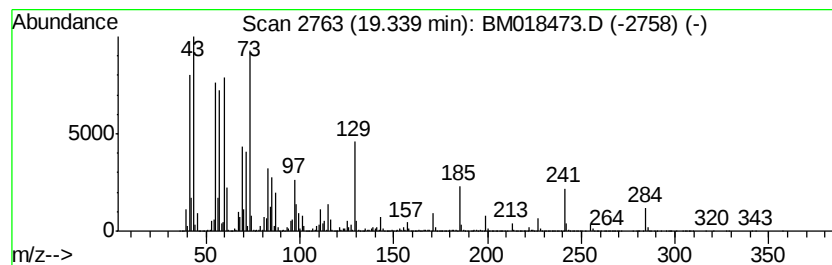
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.34	91.11 ng	28962900	Chrysene-d12	21.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	76
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018473.D
Acq On : 09 Jan 2019 15:15
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ClientSampleId :
CPSB-07(15-20)

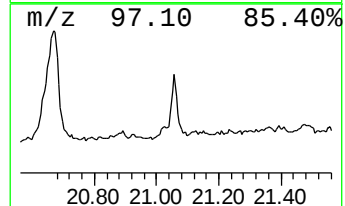
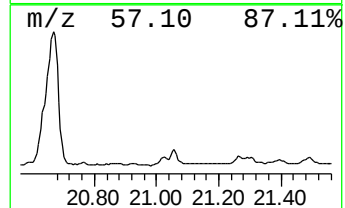
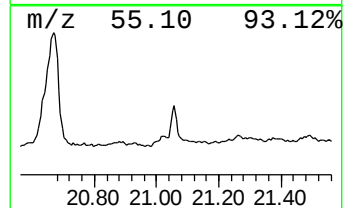
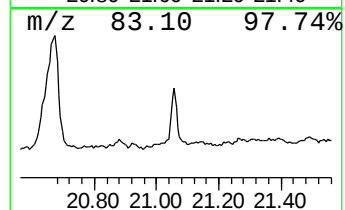
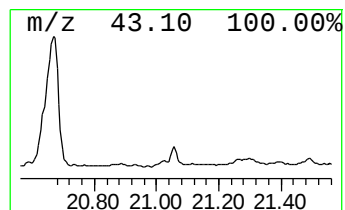
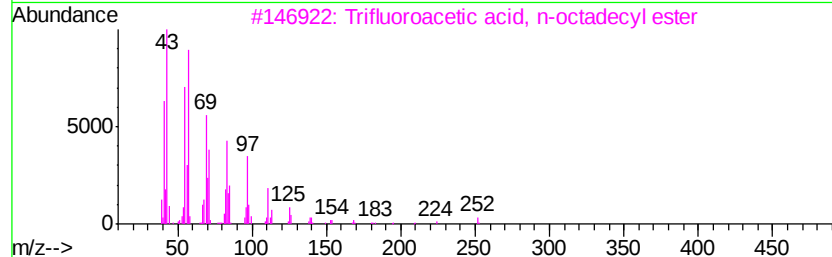
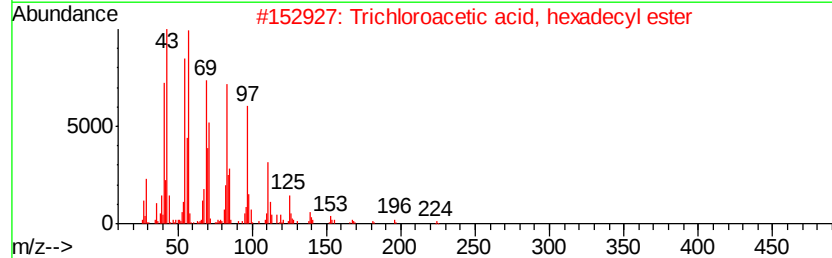
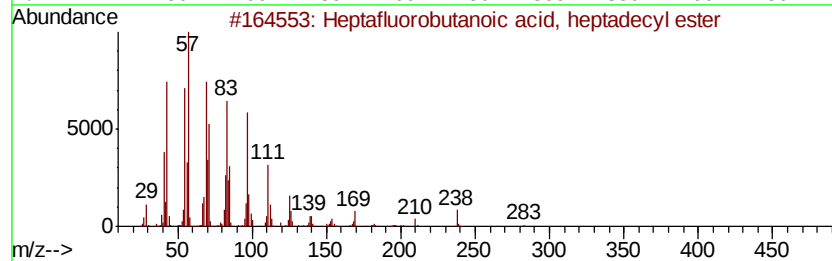
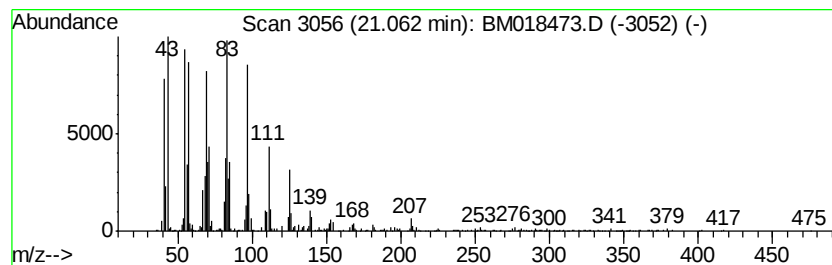
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptafluorobutanoic acid, h... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	7.28 ng	2315280	Chrysene-d12	21.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
4		1-Nonadecene	266	C19H38	018435-45-5	90
5		1-Octadecanol	270	C18H38O	000112-92-5	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018473.D
Acq On : 09 Jan 2019 15:15
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CPSB-07(15-20)

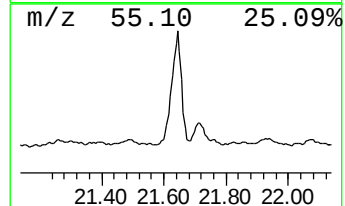
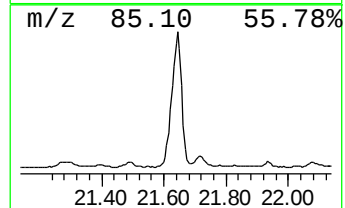
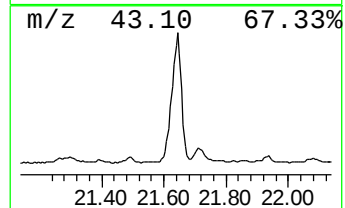
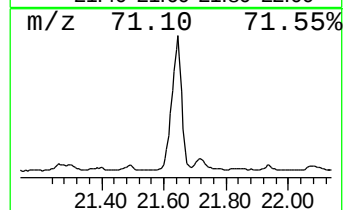
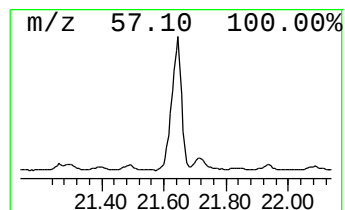
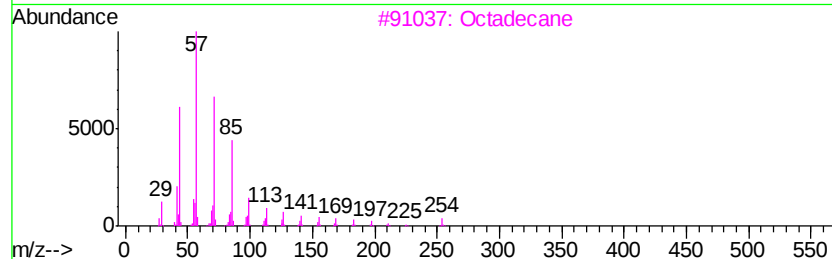
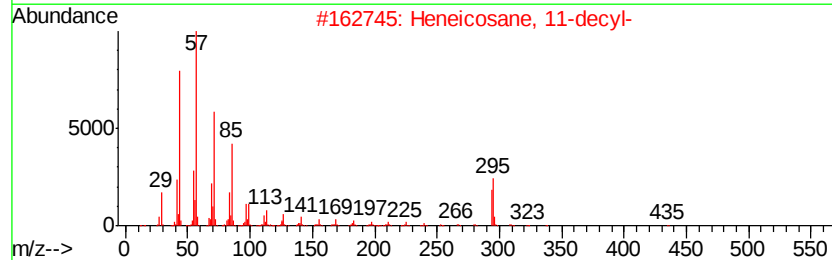
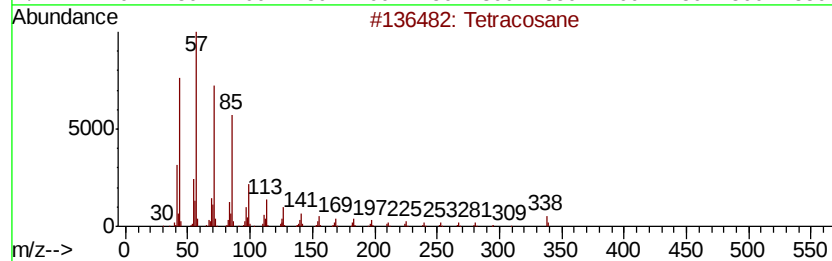
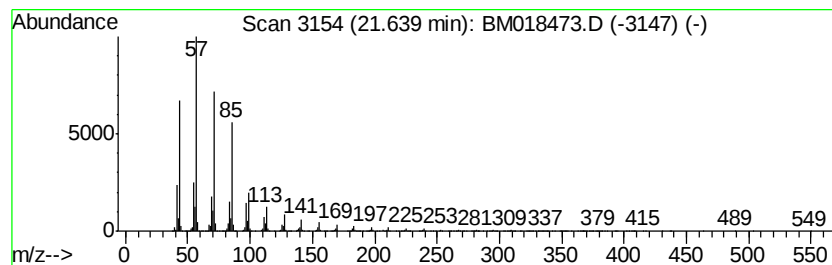
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.64	71.29 ng	22661600	Chrysene-d12	21.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	98
2		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	96
3		Octadecane	254	C18H38	000593-45-3	95
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
 Data File : BM018473.D
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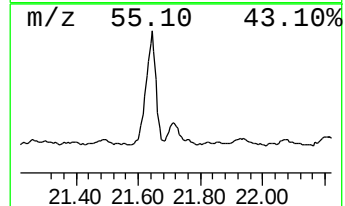
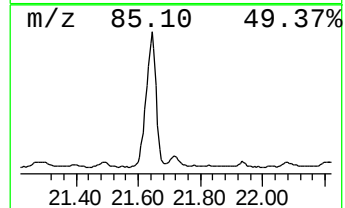
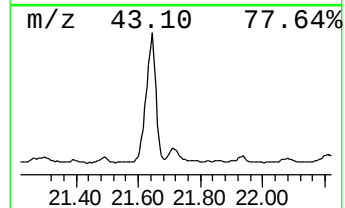
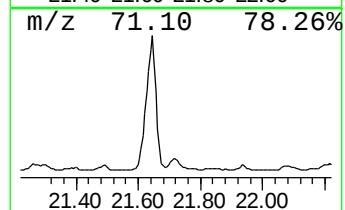
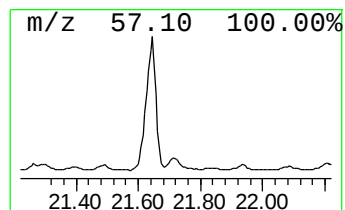
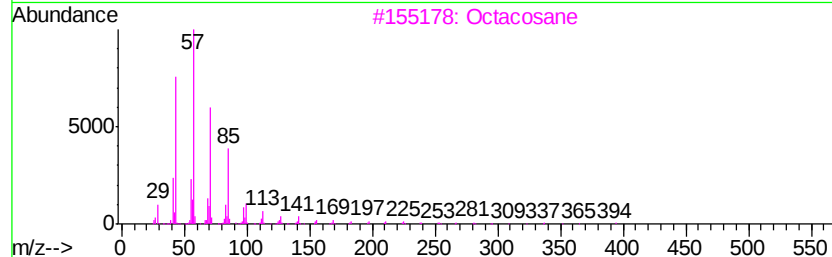
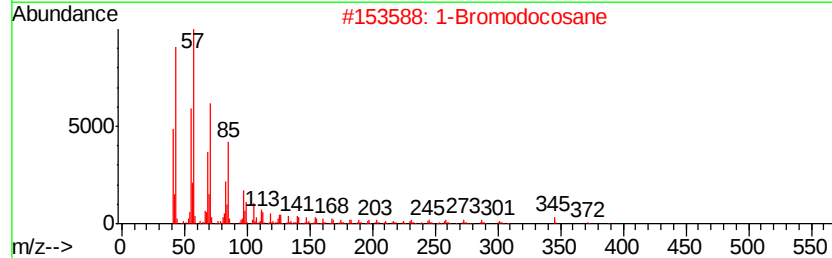
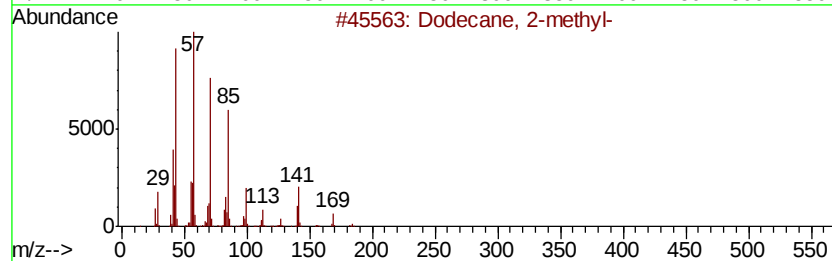
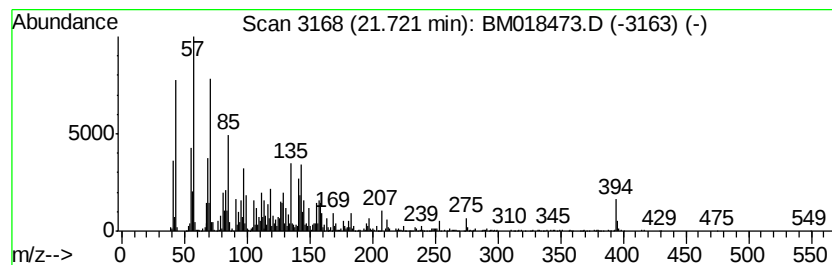
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 14 Dodecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.72	15.75 ng	5007140	Chrysene-d12	21.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	78
2		1-Bromodocosane	388	C22H45Br	006938-66-5	70
3		Octacosane	394	C28H58	000630-02-4	53
4		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	52
5		10-Methylnonadecane	282	C20H42	056862-62-5	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM010919\
Data File : BM018473.D
Acq On : 09 Jan 2019 15:15
Operator : JU/SJ
Sample : K1088-01
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CPSB-07(15-20)

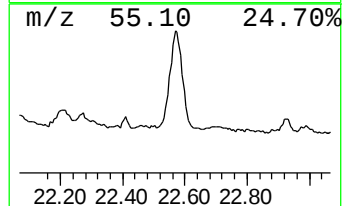
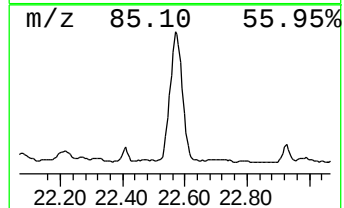
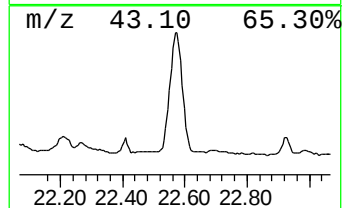
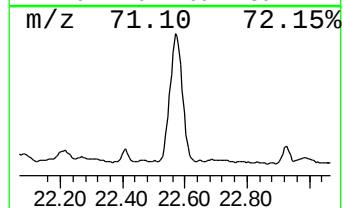
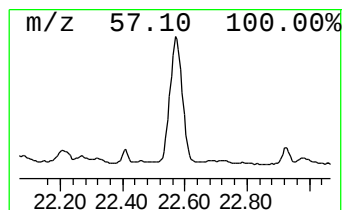
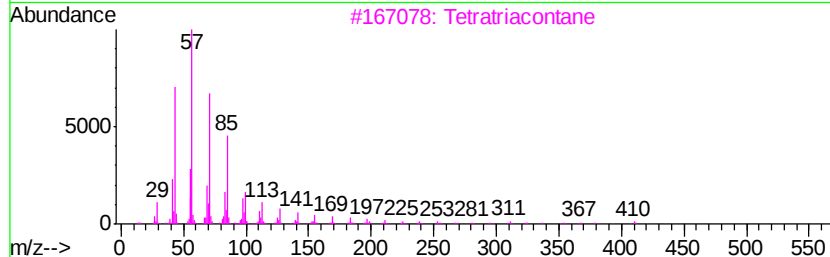
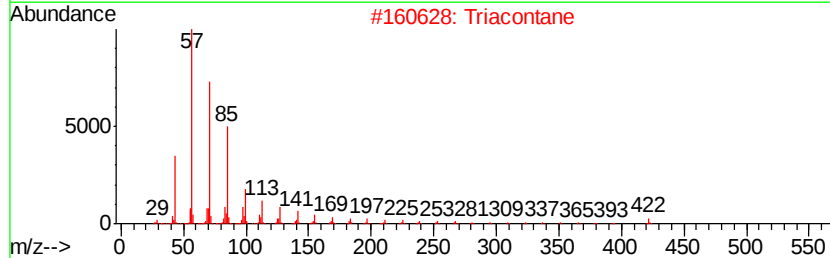
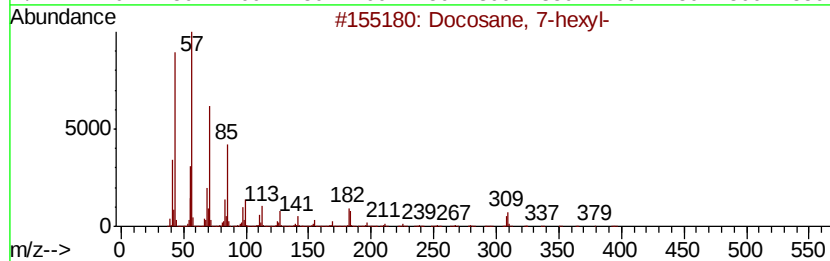
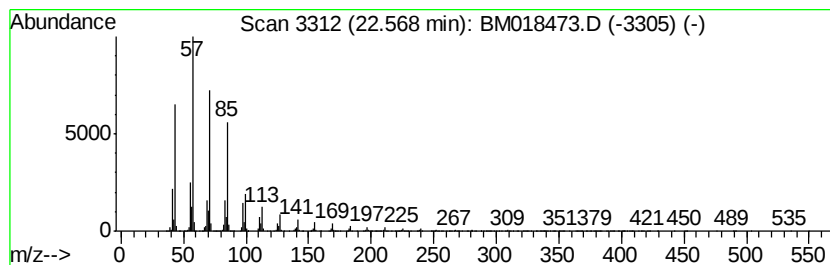
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Docosane, 7-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.57	76.02 ng	15695900	Perylene-d12	23.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
2		Triacontane	422	C30H62	000638-68-6	91
3		Tetratriacontane	479	C34H70	014167-59-0	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM010919\
 Data File : BM018473.D
 Acq On : 09 Jan 2019 15:15
 Operator : JU/SJ
 Sample : K1088-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CPSB-07(15-20)

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
3-Penten-2-one, 4...	4.30	2.2	ng	296276	1	7.76	2676300	20.0
2-Pentanone, 4-hy...	4.90	2.7	ng	362834	1	7.76	2676300	20.0
unknown7.30	7.30	67.9	ng	9087350	1	7.76	2676300	20.0
Pentadecane, 2,6,...	16.13	2.4	ng	681454	4	17.16	5726640	20.0
Tridecane	16.95	2.9	ng	827516	4	17.16	5726640	20.0
n-Hexadecanoic acid	18.07	102.5	ng	29356800	4	17.16	5726640	20.0
9-Octadecenoic ac...	19.00	2.1	ng	611753	4	17.16	5726640	20.0
Heptacosane	19.16	76.3	ng	21844300	4	17.16	5726640	20.0
Octadecanoic acid	19.34	91.1	ng	28962900	5	21.35	6357660	20.0
Heptafluorobutano...	21.06	7.3	ng	2315280	5	21.35	6357660	20.0
Tetracosane	21.64	71.3	ng	22661600	5	21.35	6357660	20.0
Dodecane, 2-methyl-	21.72	15.8	ng	5007140	5	21.35	6357660	20.0
Docosane, 7-hexyl-	22.57	76.0	ng	15695900	6	23.64	4129390	20.0