

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120519\
 Data File : BP001214.D
 Acq On : 05 Dec 2019 16:28
 Operator : JU
 Sample : K6100-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TH-9

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_P\METHODS\8270-BP112719.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	2.352	41	45	56	rVB	17834	28733	1.03%	0.113%
2	5.628	597	602	614	rVB	306410	472892	16.91%	1.859%
3	6.222	696	703	723	rBV	1958543	2421663	86.59%	9.519%
4	7.758	957	964	974	rBV	1882931	2592013	92.68%	10.189%
5	7.952	990	997	1009	rBV	2009784	2490847	89.06%	9.791%
6	8.311	1053	1058	1069	rVB	544392	610127	21.82%	2.398%
7	8.552	1093	1099	1104	rBV	1608785	1907710	68.21%	7.499%
8	9.193	1201	1208	1212	rBV	1325655	1566825	56.02%	6.159%
9	10.346	1398	1404	1411	rBV	618093	723839	25.88%	2.845%
10	12.128	1699	1707	1724	rBV	1926615	2527731	90.38%	9.936%
11	12.793	1815	1820	1832	rBV	97990	118476	4.24%	0.466%
12	13.204	1884	1890	1903	rBV	645883	807555	28.87%	3.174%
13	14.498	2103	2110	2133	rBV	1322079	1749295	62.55%	6.876%
14	15.604	2289	2298	2306	rBV	763002	865369	30.94%	3.402%
15	16.492	2445	2449	2463	rBV2	65606	92031	3.29%	0.362%
16	17.892	2681	2687	2691	rBV	2480525	2796807	100.00%	10.994%
17	18.263	2742	2750	2755	rBV	33229	44778	1.60%	0.176%
18	18.710	2822	2826	2834	rVB	35952	37827	1.35%	0.149%
19	19.128	2892	2897	2912	rBV2	193062	485357	17.35%	1.908%
20	19.245	2912	2917	2922	rVV	774112	863837	30.89%	3.396%
21	19.292	2922	2925	2931	rVB	82229	88131	3.15%	0.346%
22	19.539	2963	2967	2976	rBV	33728	45231	1.62%	0.178%
23	19.933	3030	3034	3050	rBV4	55140	116450	4.16%	0.458%
24	20.310	3094	3098	3102	rBV	64625	73929	2.64%	0.291%
25	20.704	3161	3165	3170	rBV	91461	113109	4.04%	0.445%
26	21.022	3213	3219	3231	rVV	596897	821332	29.37%	3.229%
27	21.145	3235	3240	3246	rVB2	62620	93726	3.35%	0.368%
28	21.645	3319	3325	3331	rBV	65270	109615	3.92%	0.431%
29	21.722	3331	3338	3342	rBV7	21912	60528	2.16%	0.238%
30	22.216	3417	3422	3429	rBV2	25508	47839	1.71%	0.188%
31	22.892	3531	3537	3547	rVB4	14354	34868	1.25%	0.137%
32	23.610	3653	3659	3665	rVB6	28499	64645	2.31%	0.254%
33	23.892	3700	3707	3717	rBV8	27716	109032	3.90%	0.429%
34	24.016	3718	3728	3744	rVB4	141232	457024	16.34%	1.797%

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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
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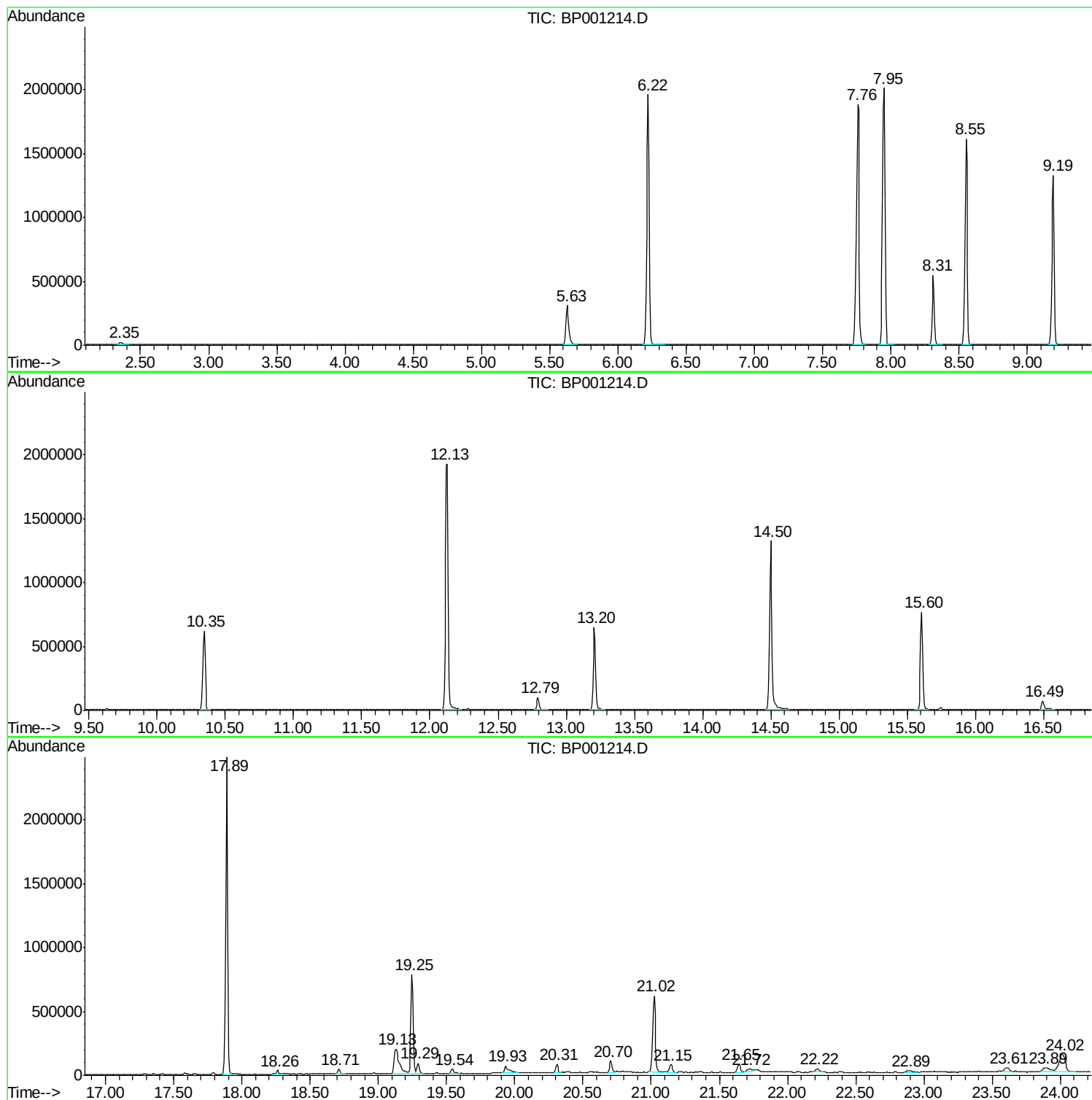
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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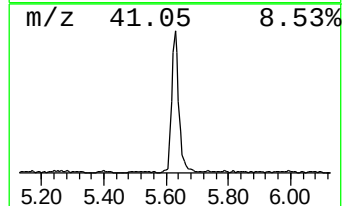
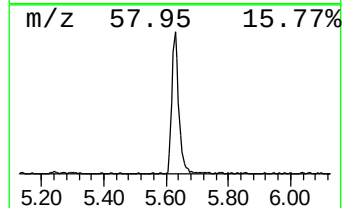
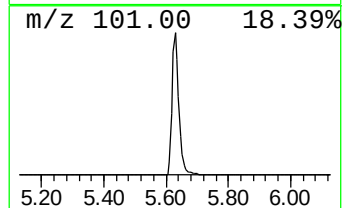
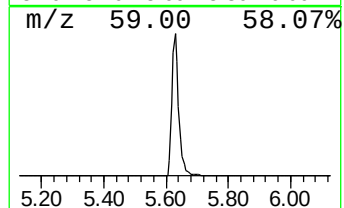
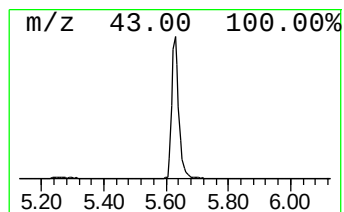
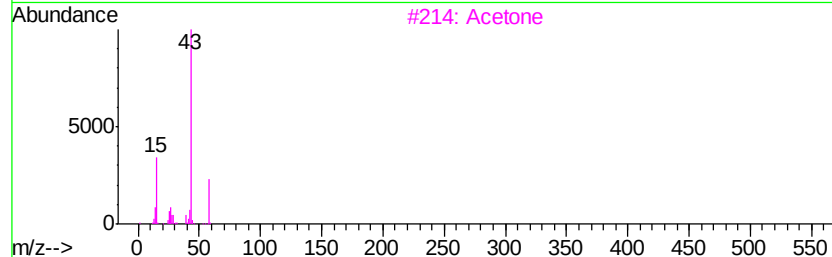
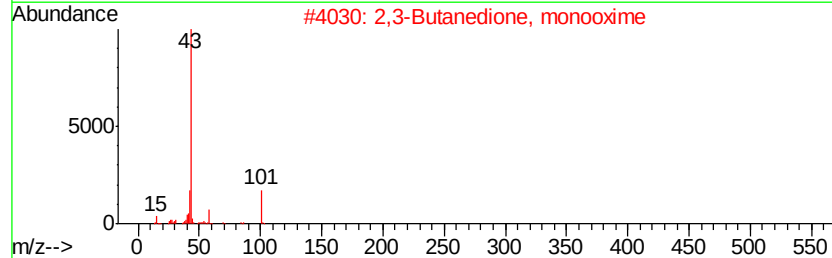
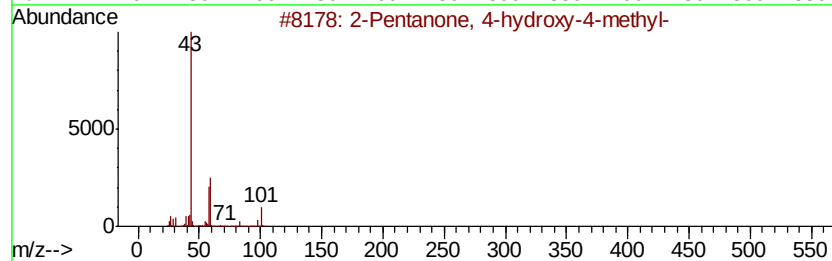
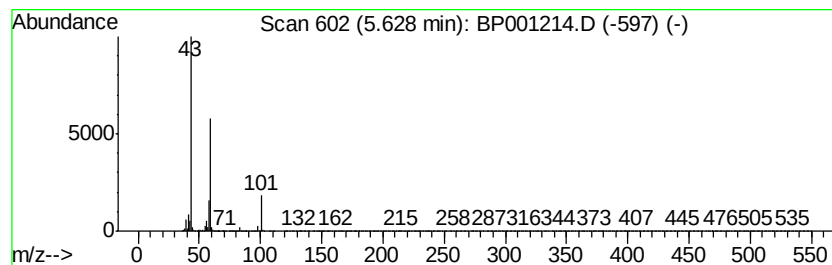
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	15.50 ng	472892	1,4-Dichlorobenzene-d4	8.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3			Acetone	58	C3H6O	000067-64-1	12
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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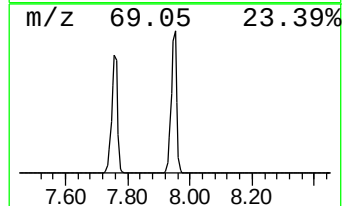
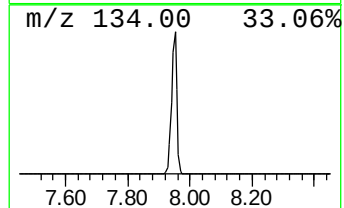
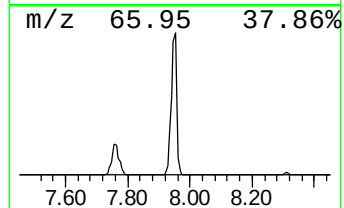
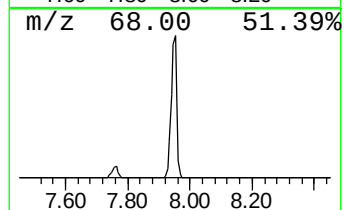
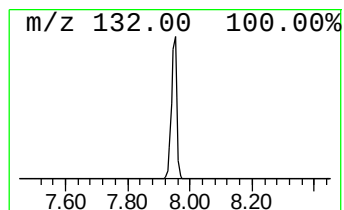
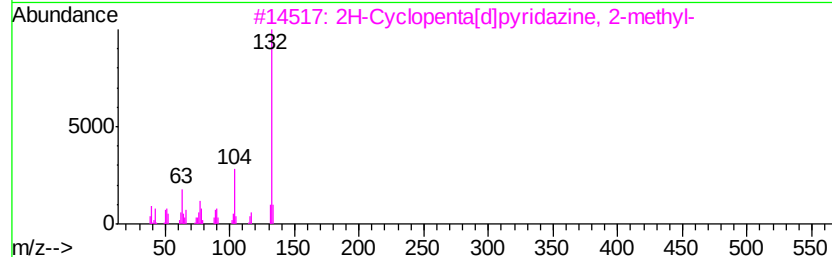
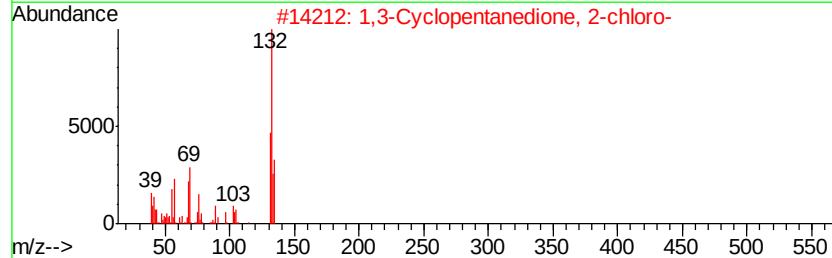
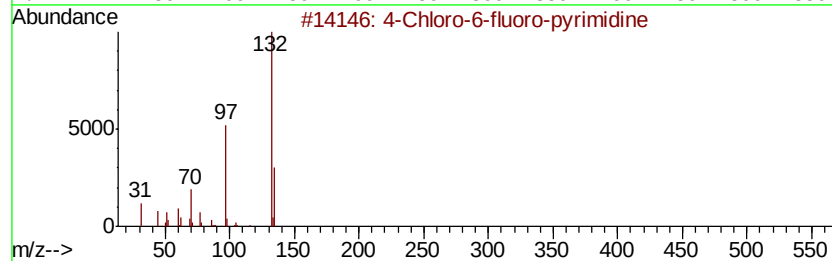
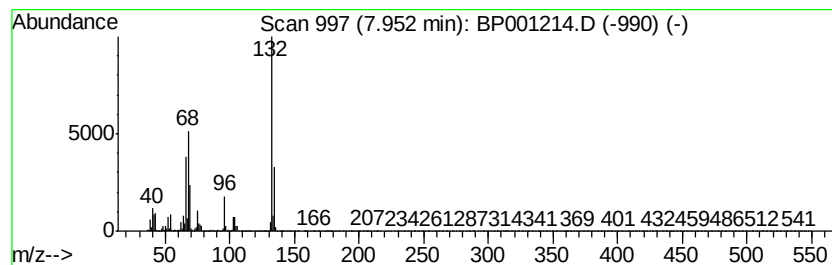
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.95 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.95	81.65 ng	2490850	1,4-Dichlorobenzene-d4	8.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3		2H-Cyclopentafldpyridazine, 2-me...	132	C8H8N2	022291-85-6	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	14



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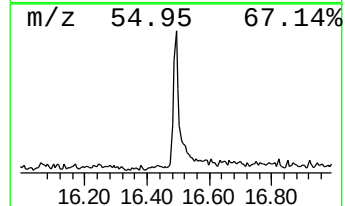
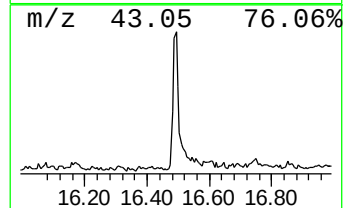
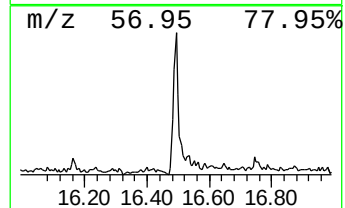
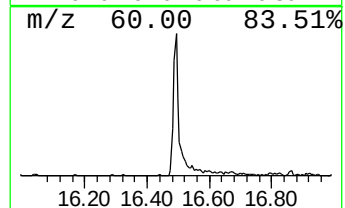
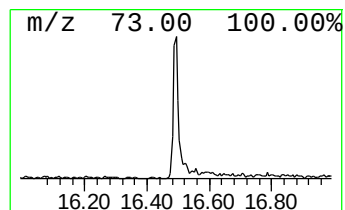
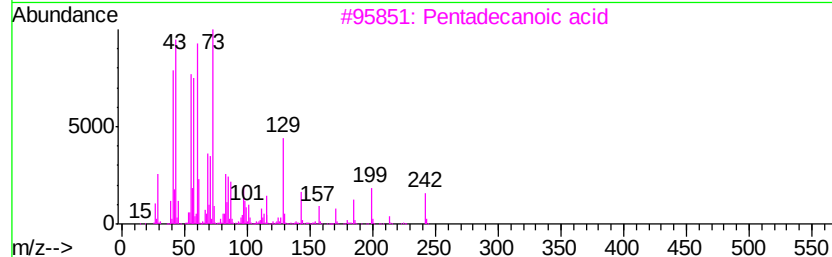
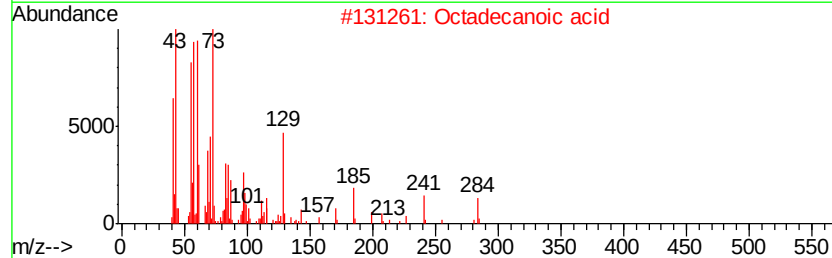
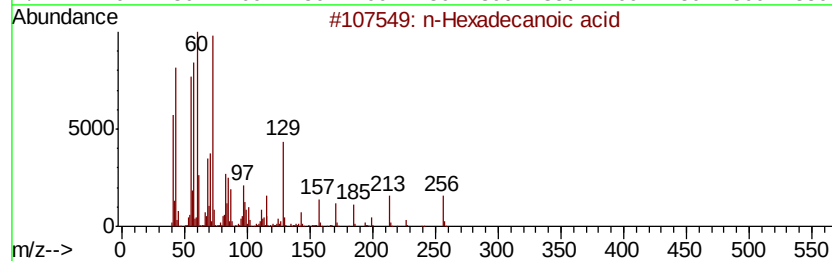
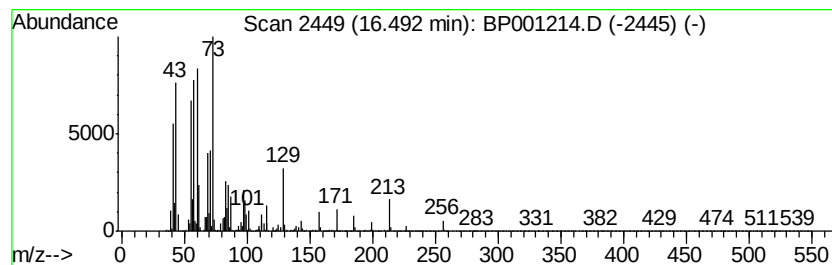
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.49	2.13 ng	92031	Phenanthrene-d10		15.60
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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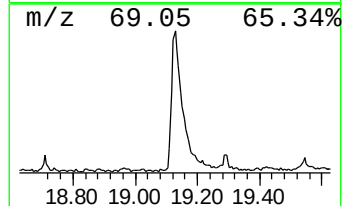
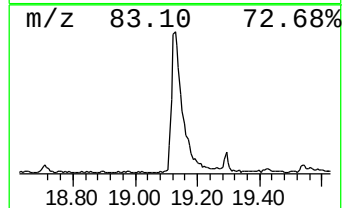
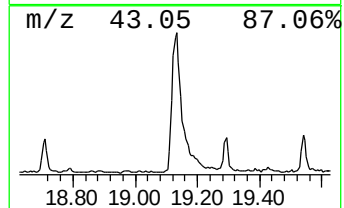
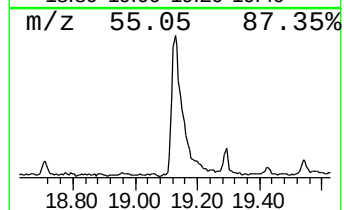
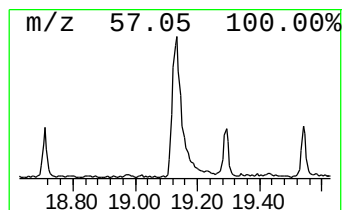
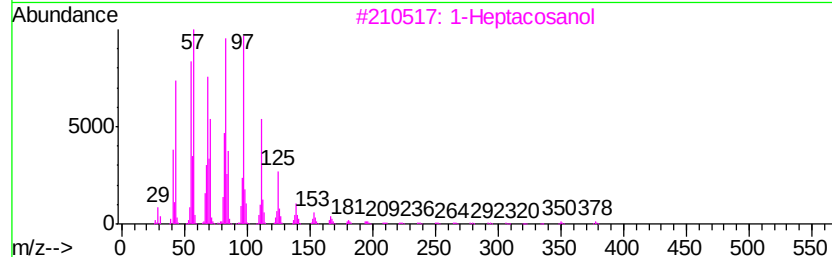
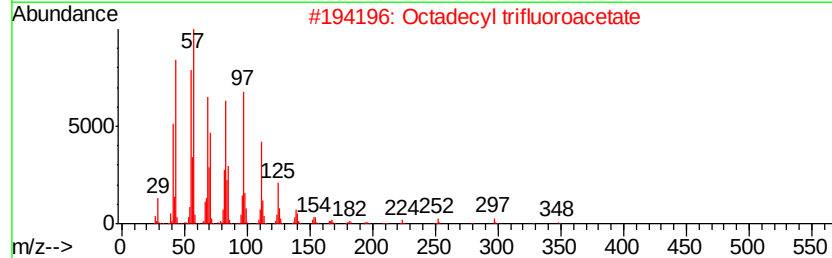
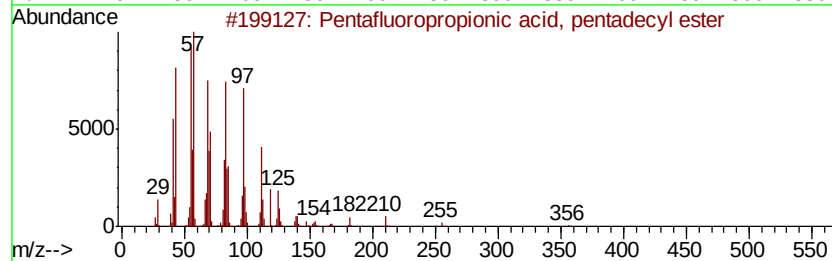
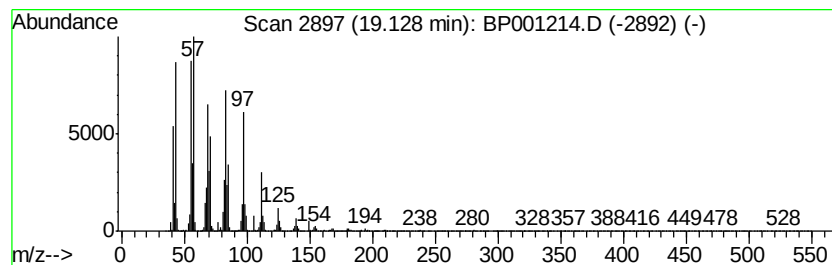
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	11.24 ng	485357	Chrysene-d12	19.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
2		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5		Octacosanol	410	C28H58O	000557-61-9	91



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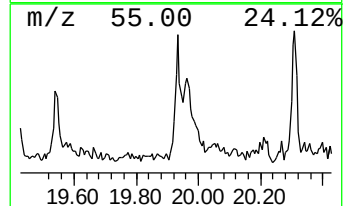
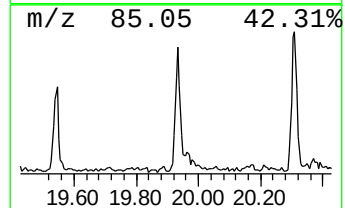
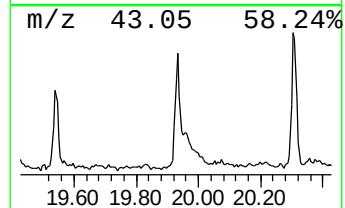
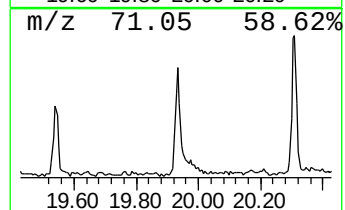
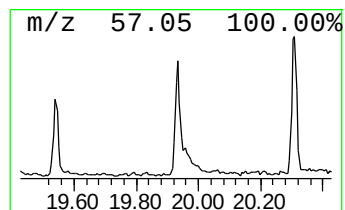
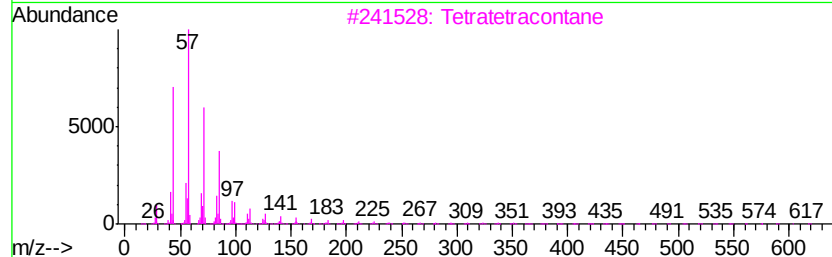
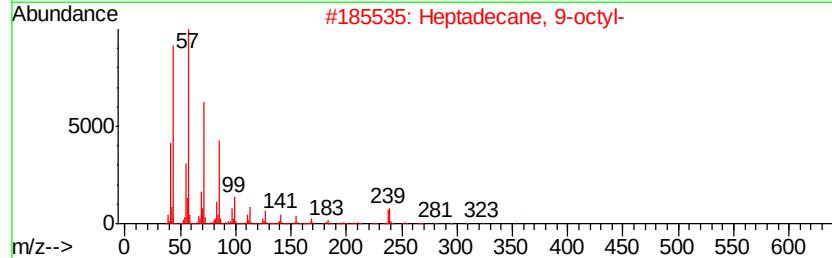
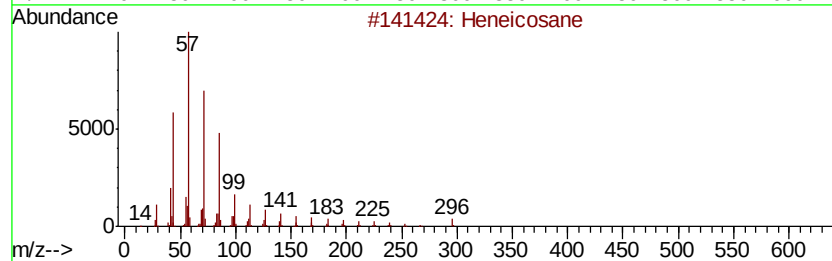
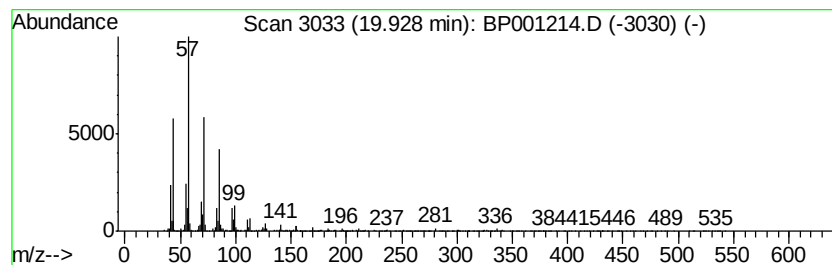
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.93	2.70 ng	116450	Chrysene-d12	19.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heneicosane	296 C21H44	000629-94-7	96
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	95
3	Tetratetracontane	619 C44H90	007098-22-8	91
4	Docosane	310 C22H46	000629-97-0	91
5	Octacosane	394 C28H58	000630-02-4	91



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TH-9

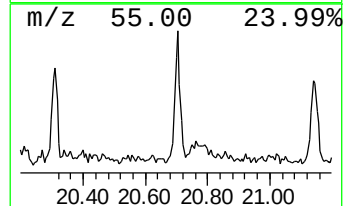
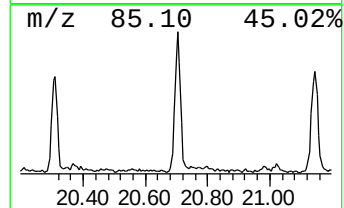
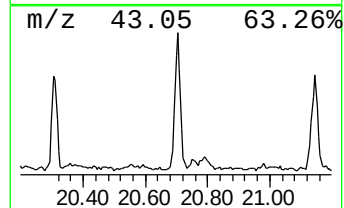
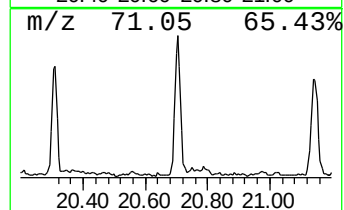
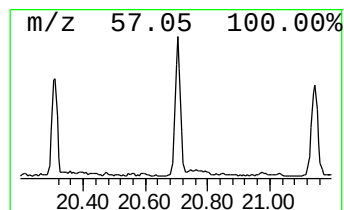
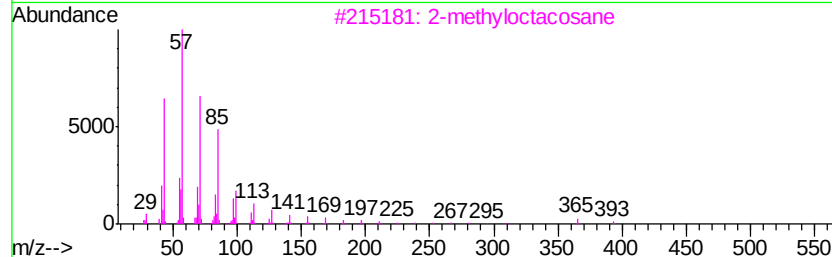
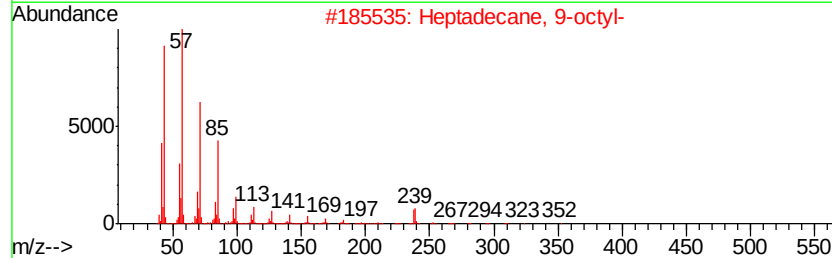
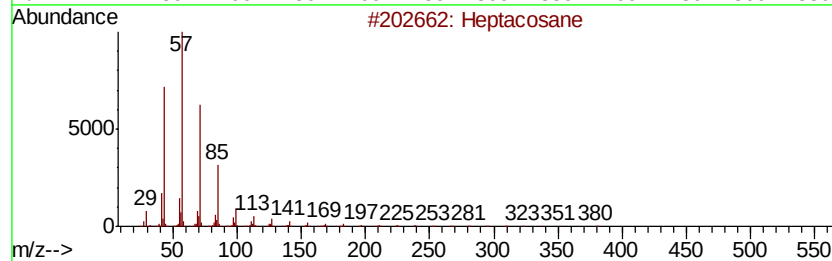
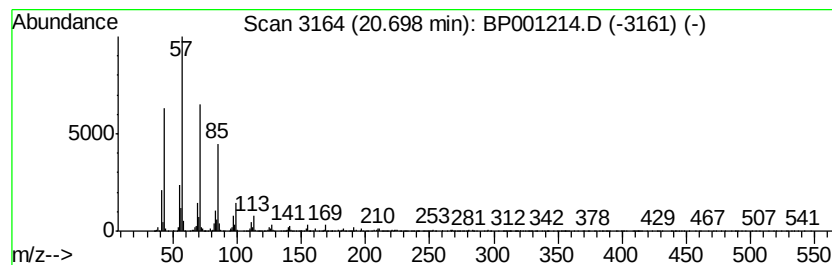
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.70	2.75 ng	113109	Perylene-d12	21.02

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane		380	C27H56	000593-49-7	91
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	90
4	Tetracosane		338	C24H50	000646-31-1	90
5	Tetratetracontane		619	C44H90	007098-22-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120519\
Data File : BP001214.D
Acq On : 05 Dec 2019 16:28
Operator : JU
Sample : K6100-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TH-9

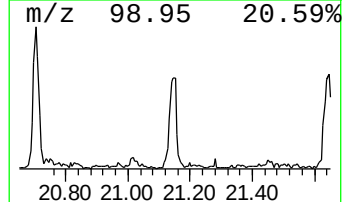
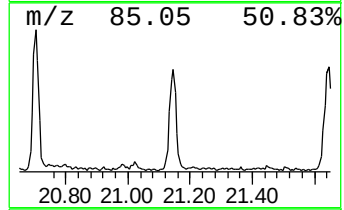
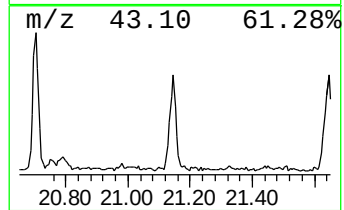
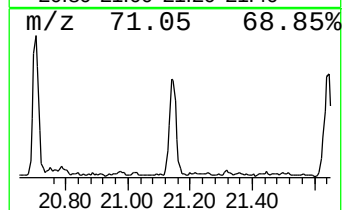
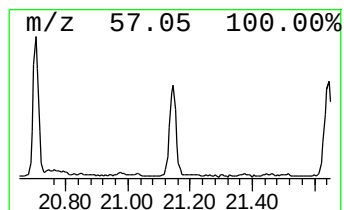
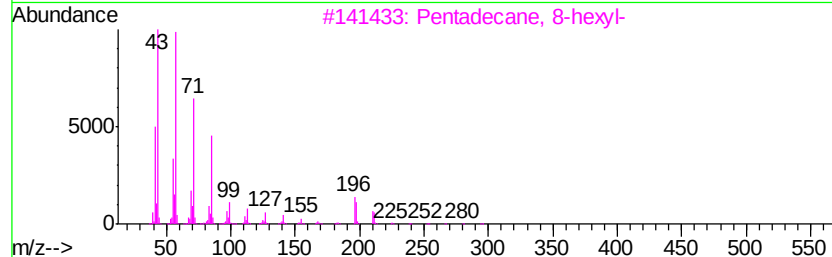
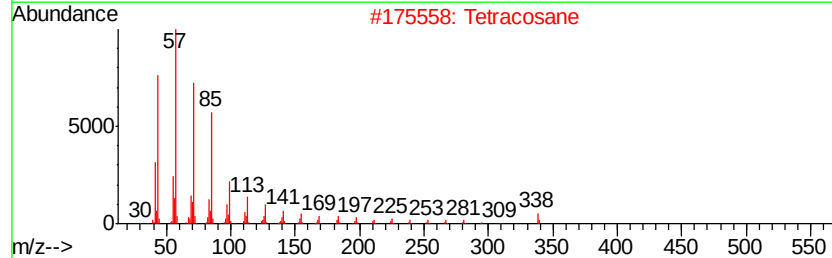
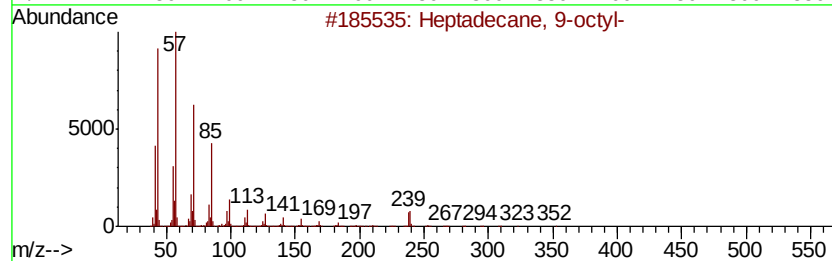
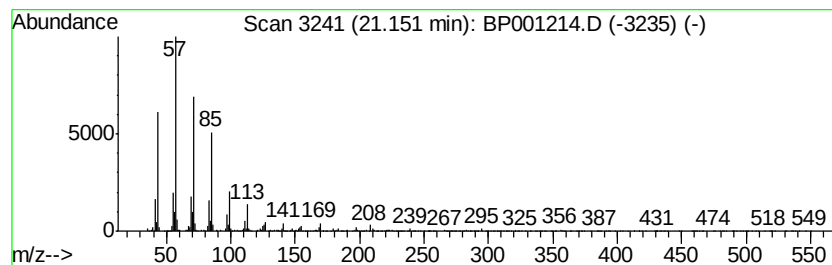
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.15	2.28 ng	93726	Perylene-d12	21.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	97
2		Tetracosane	338	C24H50	000646-31-1	95
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120519\
Data File : BP001214.D
Acq On : 05 Dec 2019 16:28
Operator : JU
Sample : K6100-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

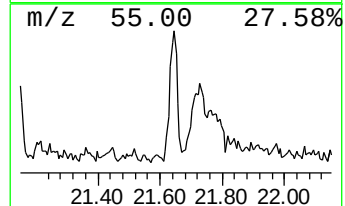
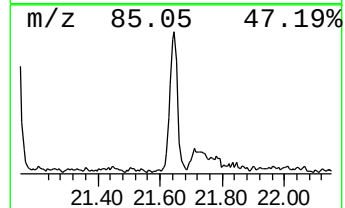
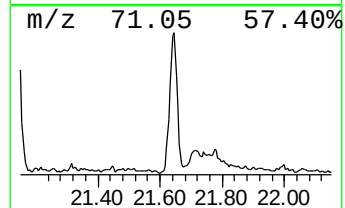
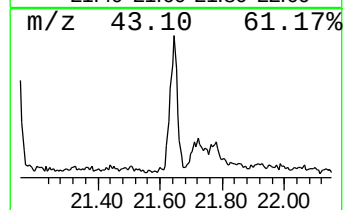
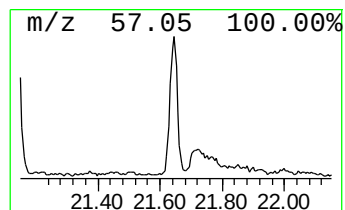
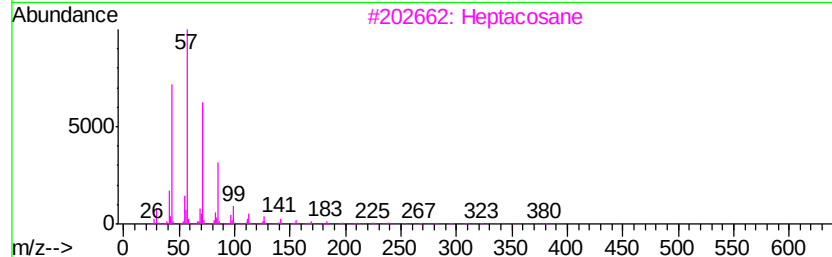
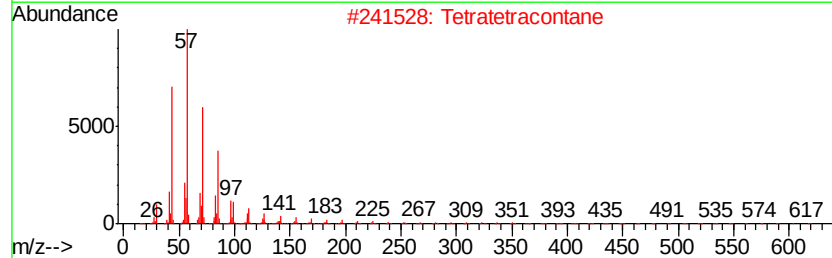
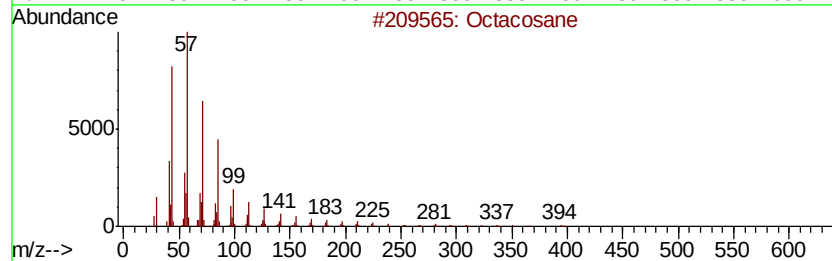
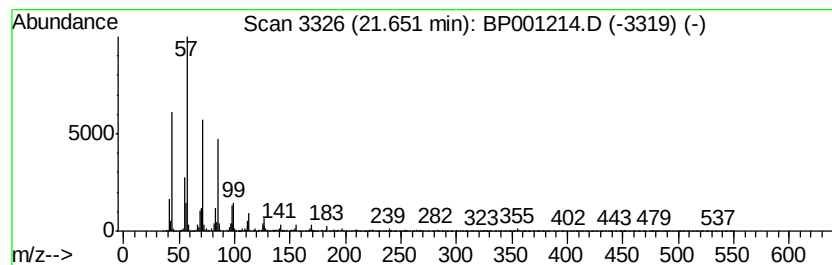
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.65	2.67 ng	109615	Perylene-d12	21.02
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394	C28H58	000630-02-4 91
2	Tetratetracontane	619	C44H90	007098-22-8 91
3	Heptacosane	380	C27H56	000593-49-7 91
4	Tetracosane	338	C24H50	000646-31-1 87
5	Hexadecane	226	C16H34	000544-76-3 87



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120519\
Data File : BP001214.D
Acq On : 05 Dec 2019 16:28
Operator : JU
Sample : K6100-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

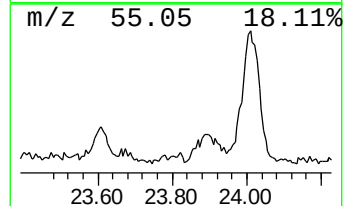
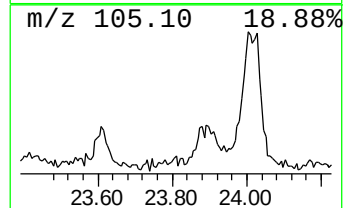
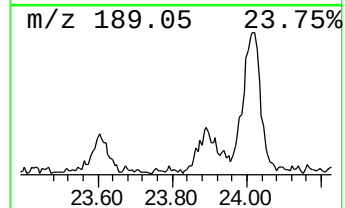
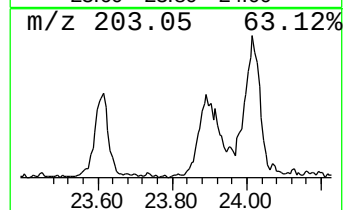
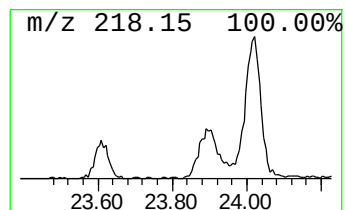
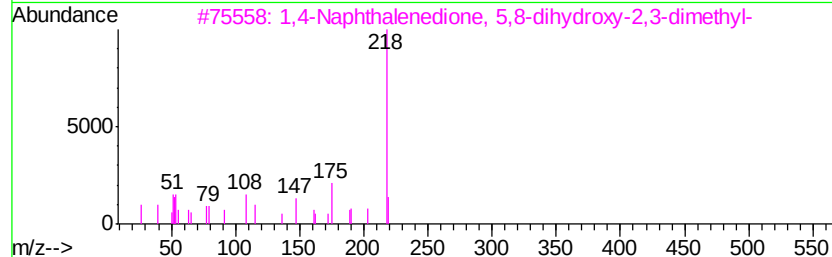
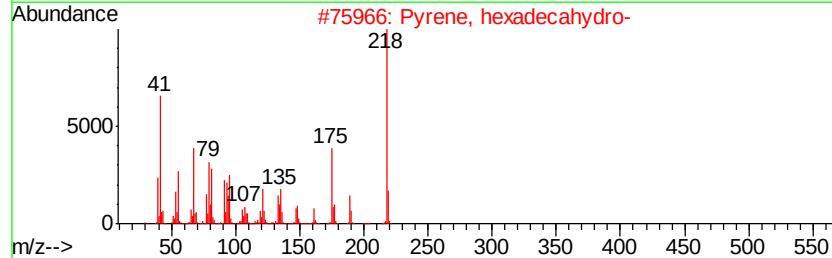
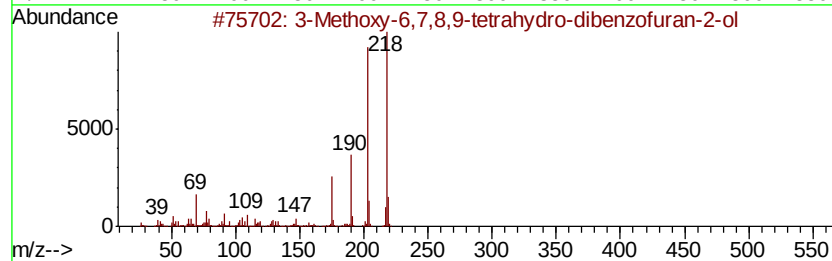
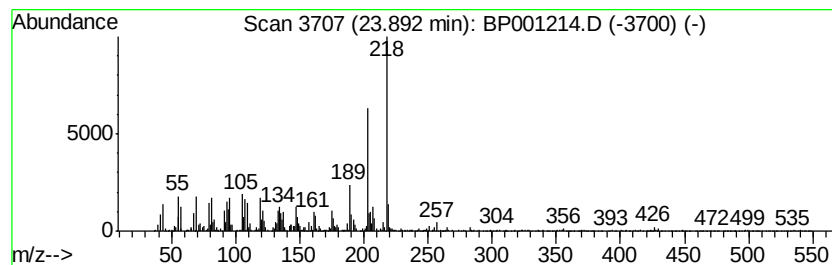
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 3-Methoxy-6,7,8,9-tetrahydr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
23.89	2.66 ng	109032	Perylene-d12	21.02		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	64
2		Pyrene, hexadecahydro-	218	C16H26	002435-85-0	60
3		1,4-Naphthalenedione, 5,8-dihydr...	218	C12H10O4	021418-10-0	53
4		Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	52
5		5-Adamantan-1-yl-2H-pyrazol-3-ol	218	C13H18N2O	1000274-32-3	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP120519\
Data File : BP001214.D
Acq On : 05 Dec 2019 16:28
Operator : JU
Sample : K6100-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.63	15.5	ng	472892	1	8.31	610127	20.0
unknown7.95	7.95	81.7	ng	2490850	1	8.31	610127	20.0
n-Hexadecanoic acid	16.49	2.1	ng	92031	4	15.60	865369	20.0
Pentafluoropropio...	19.13	11.2	ng	485357	5	19.25	863837	20.0
Heneicosane	19.93	2.7	ng	116450	5	19.25	863837	20.0
Heptacosane	20.70	2.8	ng	113109	6	21.02	821332	20.0
Heptadecane, 9-oc...	21.15	2.3	ng	93726	6	21.02	821332	20.0
Octacosane	21.65	2.7	ng	109615	6	21.02	821332	20.0
3-Methoxy-6,7,8,9...	23.89	2.7	ng	109032	6	21.02	821332	20.0
4,4,6a,6b,8a,11,1...	24.02	11.1	ng	457024	6	21.02	821332	20.0