

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP121119\
 Data File : BP001319.D
 Acq On : 11 Dec 2019 18:58
 Operator : JU
 Sample : K6204-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 K072-AB-WC-1

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	5.622	593	601	614	rBV	222213	358088	16.69%	1.989%
2	6.216	696	702	717	rBV	1226833	1556819	72.58%	8.646%
3	7.758	957	964	978	rBV	1330358	1673633	78.03%	9.295%
4	7.946	990	996	1010	rVB	1374458	1681220	78.38%	9.337%
5	8.305	1052	1057	1067	rVB	423933	481160	22.43%	2.672%
6	8.546	1092	1098	1103	rBV	1131568	1292484	60.26%	7.178%
7	9.187	1200	1207	1211	rBV	880496	1068732	49.82%	5.936%
8	10.340	1397	1403	1414	rBV	475314	567208	26.44%	3.150%
9	12.116	1698	1705	1723	rBV	1583663	1968261	91.76%	10.931%
10	12.787	1814	1819	1827	rBV	51447	65599	3.06%	0.364%
11	13.198	1883	1889	1896	rBV	537402	669253	31.20%	3.717%
12	14.492	2103	2109	2129	rBV	1058673	1345255	62.72%	7.471%
13	15.598	2287	2297	2301	rBV	601156	712734	33.23%	3.958%
14	15.628	2301	2302	2308	rVB	28419	28630	1.33%	0.159%
15	16.486	2444	2448	2456	rBV4	51520	79646	3.71%	0.442%
16	17.339	2589	2593	2598	rBV	57593	64398	3.00%	0.358%
17	17.645	2640	2645	2649	rBV	55340	63539	2.96%	0.353%
18	17.881	2679	2685	2689	rBV	2027853	2144977	100.00%	11.913%
19	19.145	2893	2900	2910	rBV7	60243	238306	11.11%	1.324%
20	19.239	2910	2916	2920	rVV	565405	682588	31.82%	3.791%
21	19.269	2920	2921	2926	rVB	30852	24307	1.13%	0.135%
22	19.528	2962	2965	2969	rVB	39423	38635	1.80%	0.215%
23	19.922	3028	3032	3037	rVB	51861	58898	2.75%	0.327%
24	20.292	3091	3095	3100	rVB	71683	80160	3.74%	0.445%
25	20.522	3130	3134	3145	rBV3	20289	51292	2.39%	0.285%
26	20.686	3158	3162	3167	rBV	81931	97249	4.53%	0.540%
27	20.933	3200	3204	3210	rBV	17338	25878	1.21%	0.144%
28	21.010	3211	3217	3227	rVV	401140	573910	26.76%	3.187%
29	21.122	3231	3236	3242	rVB	69435	102056	4.76%	0.567%
30	21.622	3315	3321	3329	rVB2	56489	98190	4.58%	0.545%
31	21.757	3338	3344	3350	rBV10	12577	39729	1.85%	0.221%
32	22.192	3413	3418	3424	rVB3	24588	45852	2.14%	0.255%
33	22.851	3526	3530	3537	rVB5	11761	27056	1.26%	0.150%

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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K072-AB-WC-1

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
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

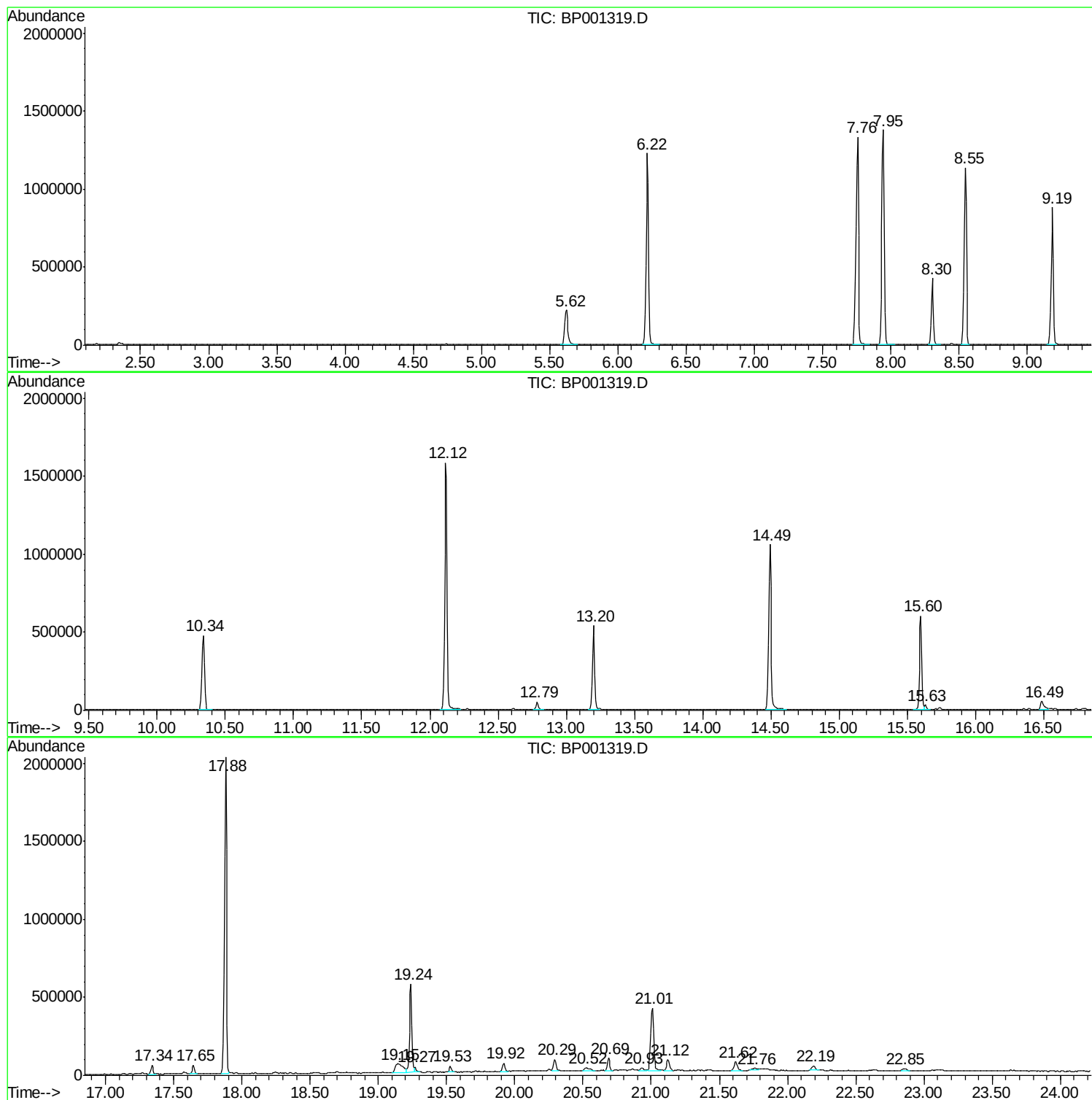
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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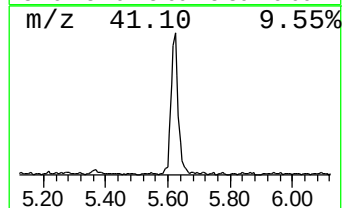
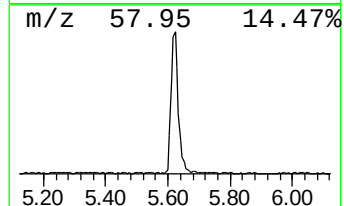
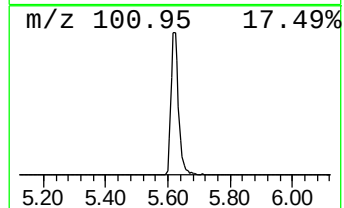
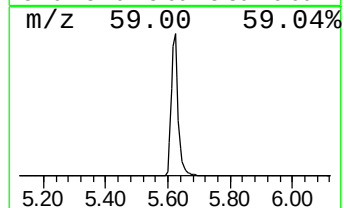
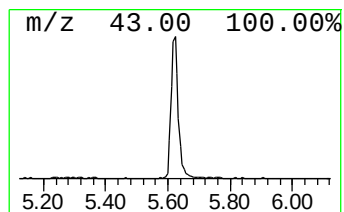
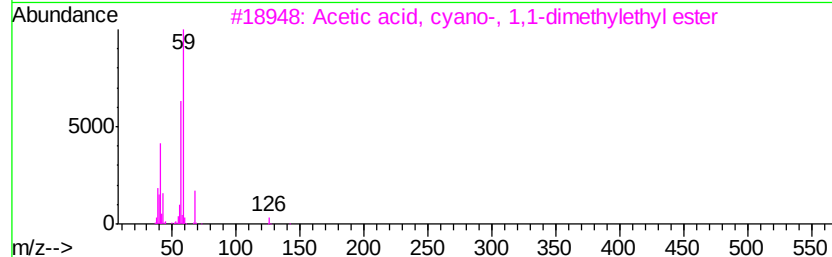
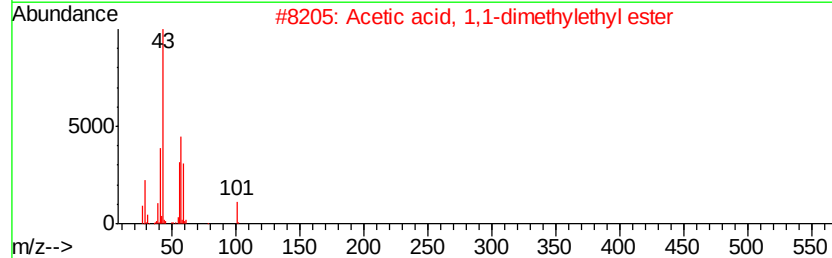
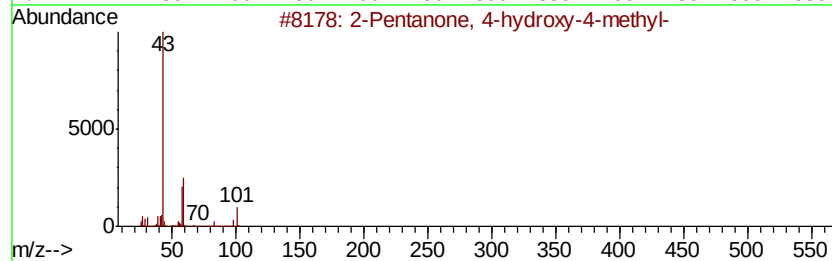
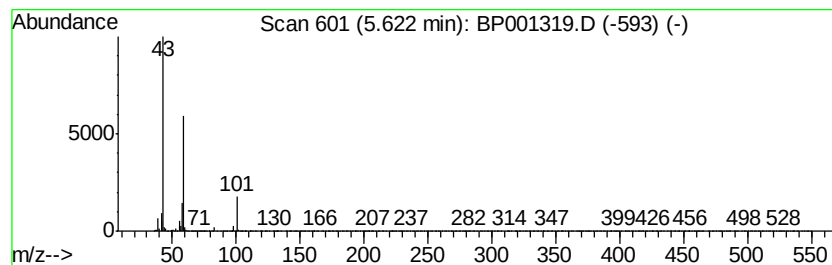
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.62	14.88 ng	358088	1,4-Dichlorobenzene-d4	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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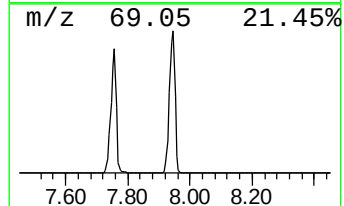
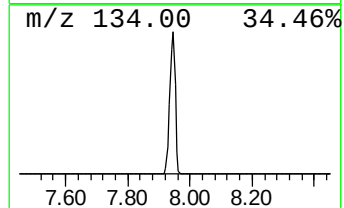
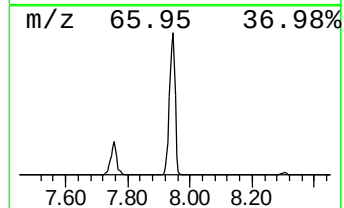
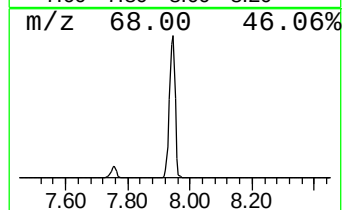
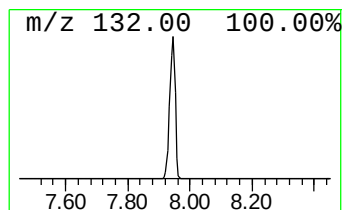
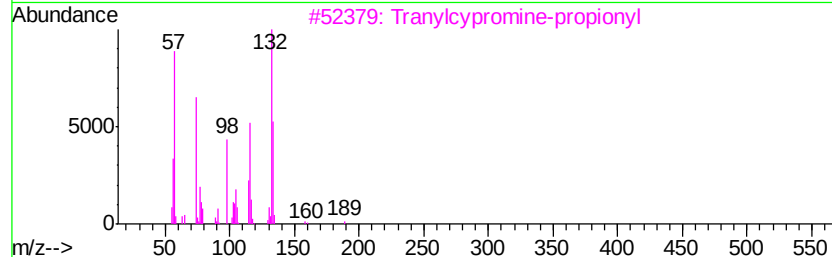
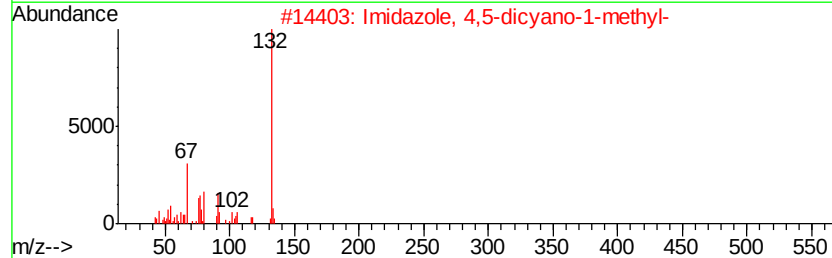
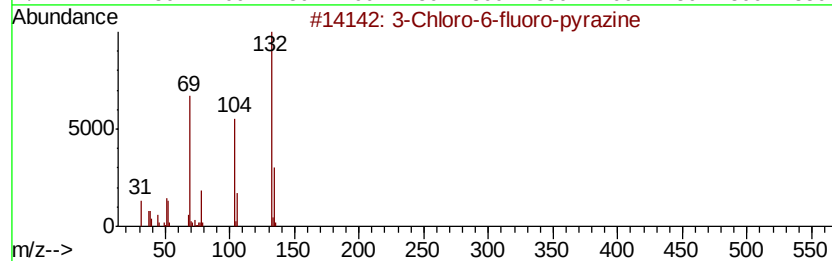
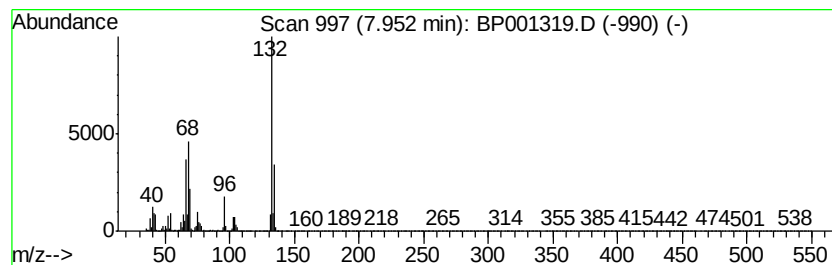
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.95 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.95	69.88 ng	1681220	1,4-Dichlorobenzene-d4	8.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		2H-Cyclopentafldpyridazine, 2-me...	132	C8H8N2	022291-85-6	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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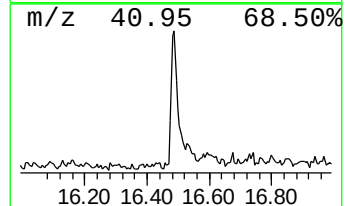
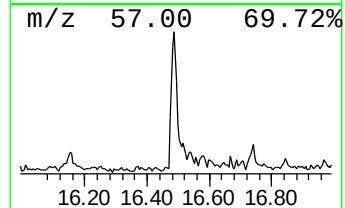
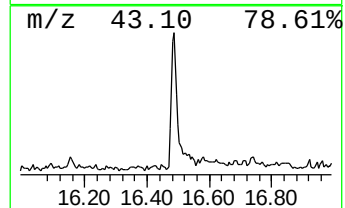
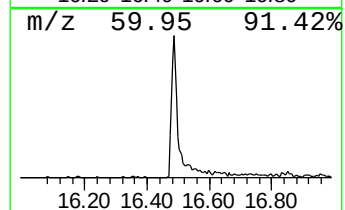
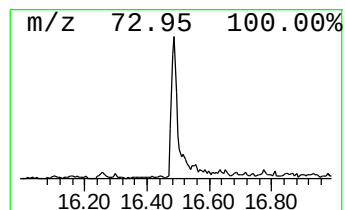
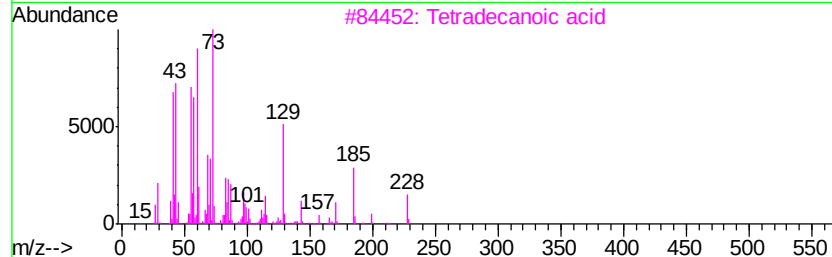
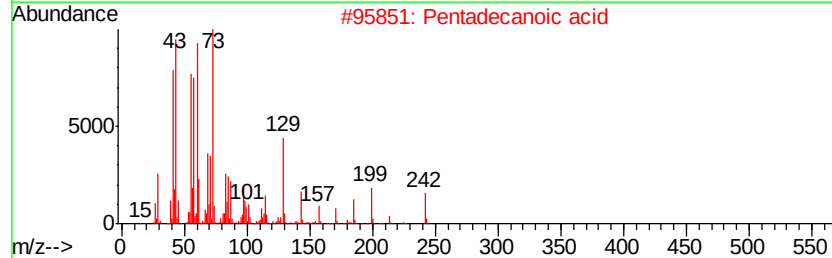
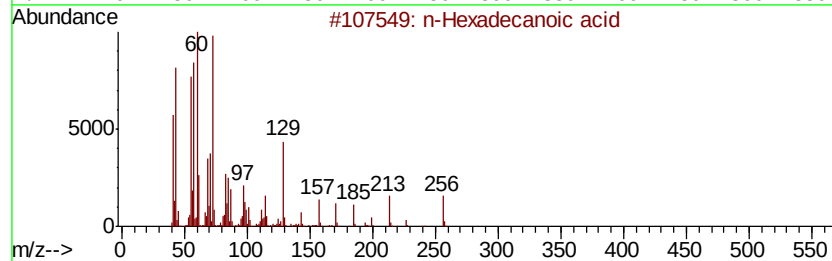
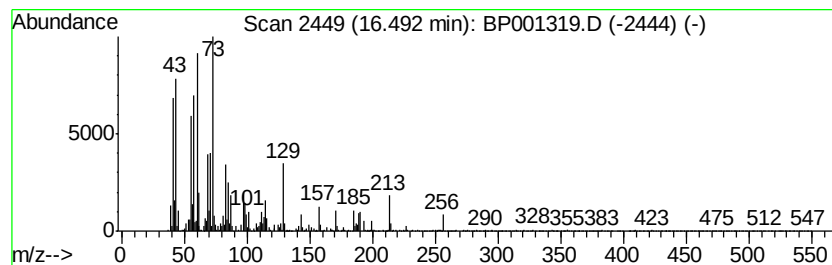
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.23 ng	79646	Phenanthrene-d10	15.60

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	90
5		n-Decanoic acid	172	C10H20O2	000334-48-5	81



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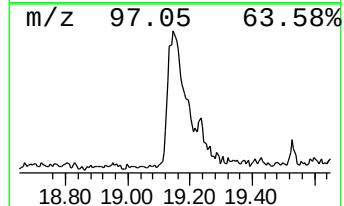
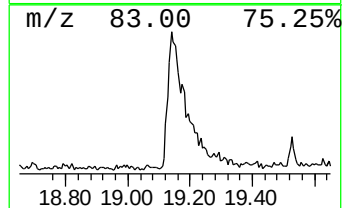
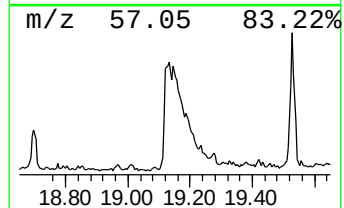
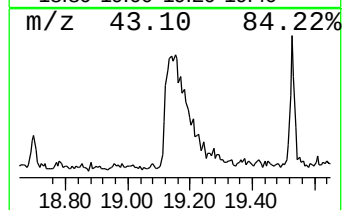
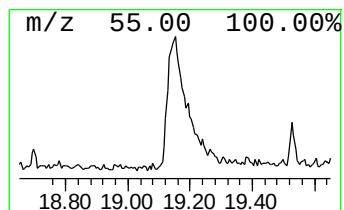
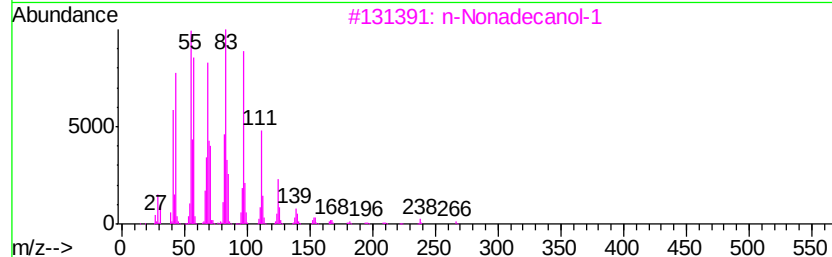
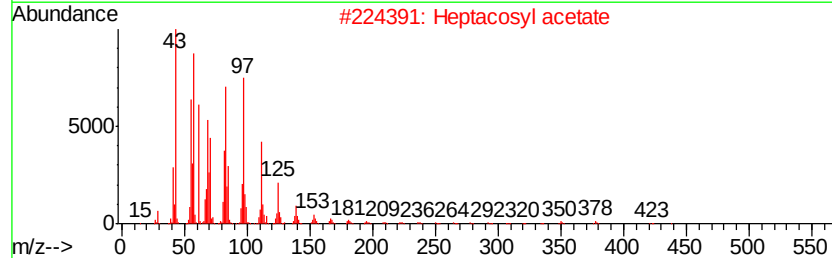
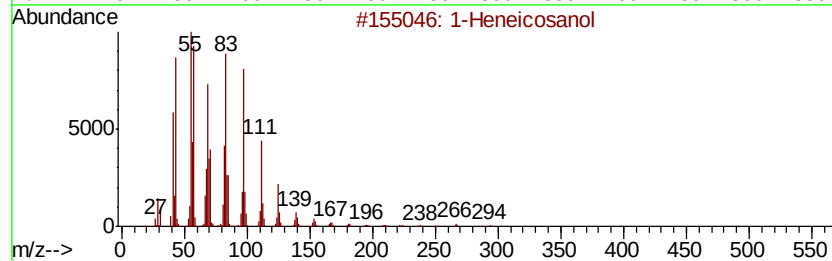
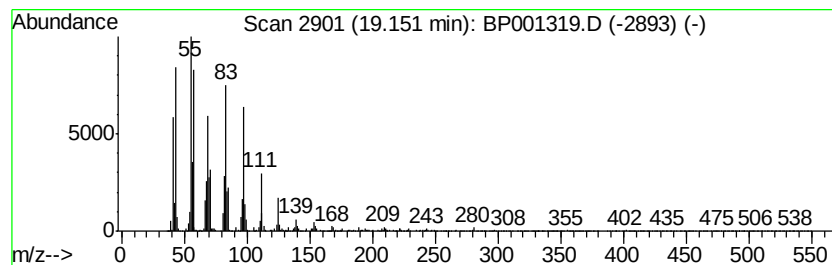
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.15	6.98 ng	238306	Chrysene-d12	19.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Heptacosyl acetate	438	C29H58O2	1000351-78-2	93
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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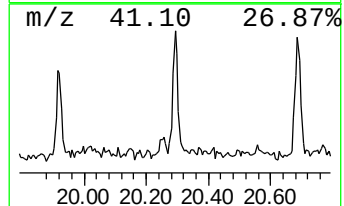
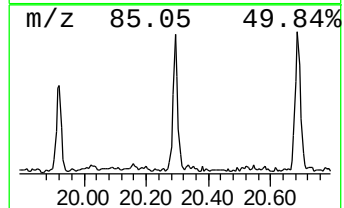
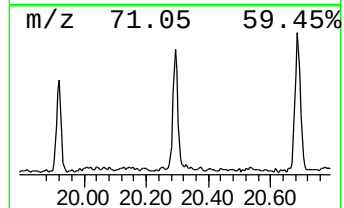
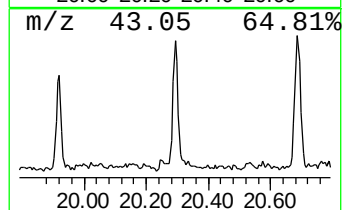
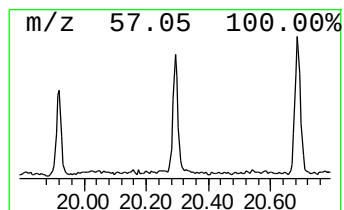
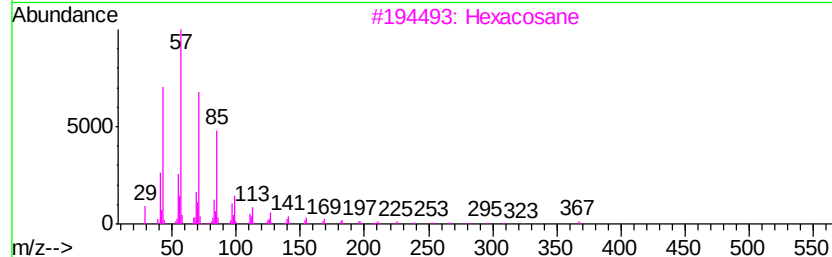
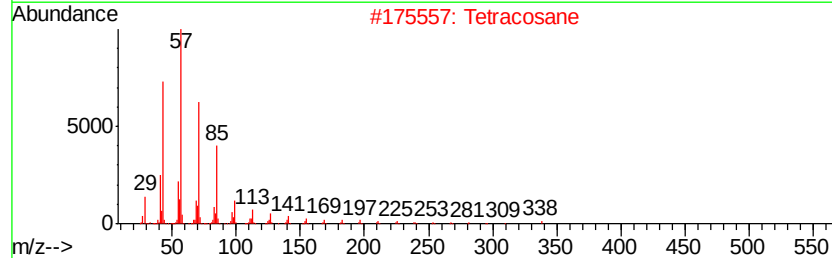
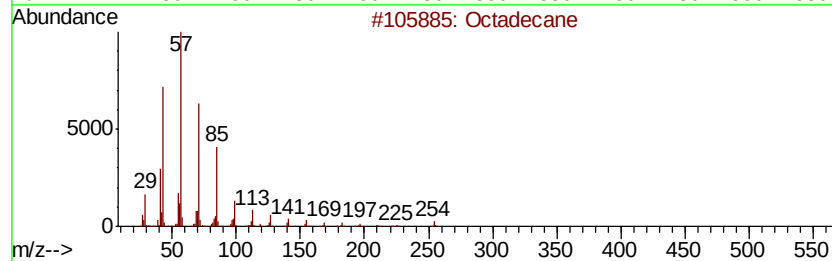
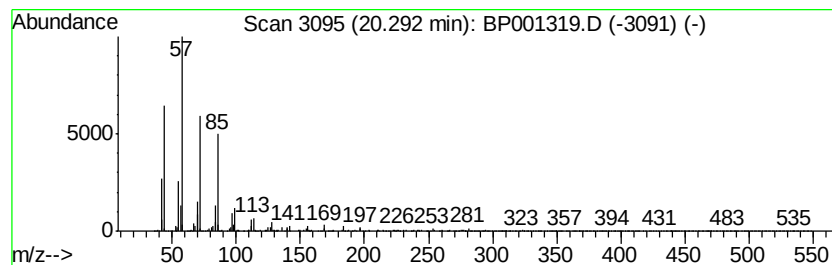
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	2.79 ng	80160	Perylene-d12	21.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	93
2		Tetracosane	338	C24H50	000646-31-1	93
3		Hexacosane	366	C26H54	000630-01-3	91
4		Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	83
5		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	81



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K072-AB-WC-1

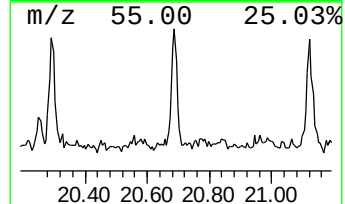
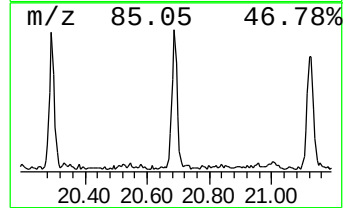
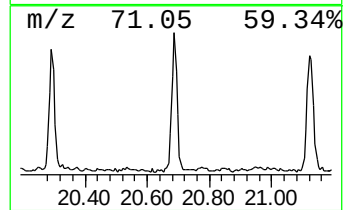
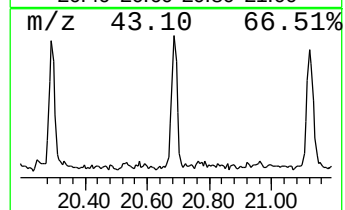
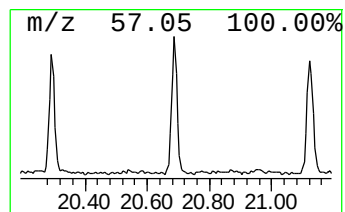
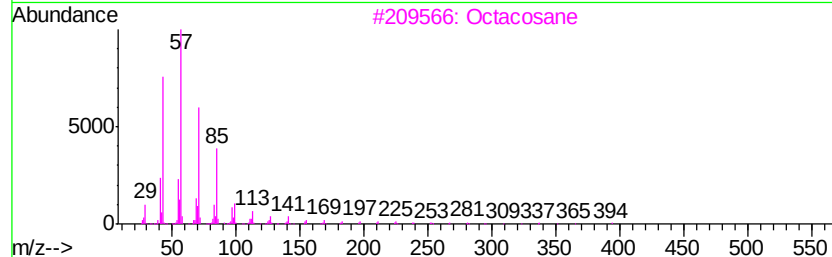
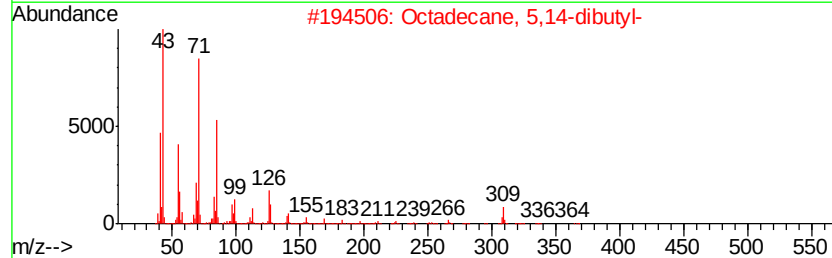
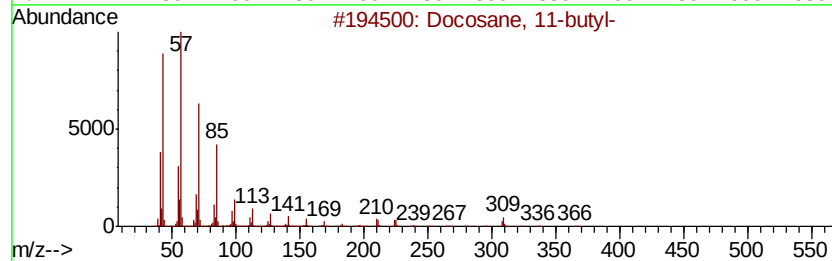
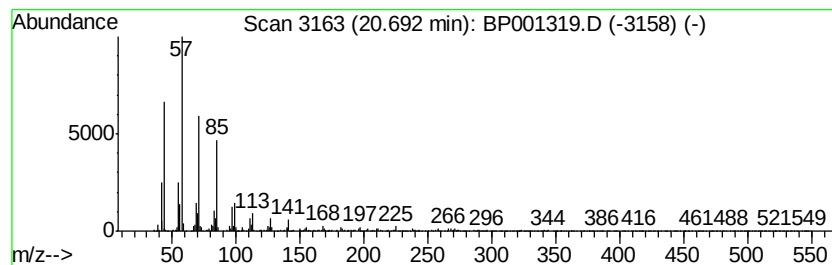
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Docosane, 11-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	3.39 ng	97249	Perylene-d12	21.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 11-butyl-	366	C26H54	013475-76-8	94
2		Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	93
3		Octacosane	394	C28H58	000630-02-4	91
4		Hexacosane	366	C26H54	000630-01-3	91
5		Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP121119\
Data File : BP001319.D
Acq On : 11 Dec 2019 18:58
Operator : JU
Sample : K6204-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K072-AB-WC-1

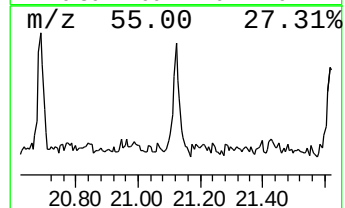
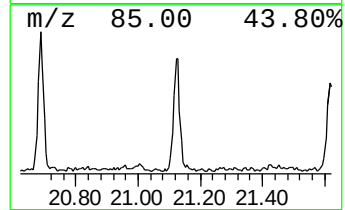
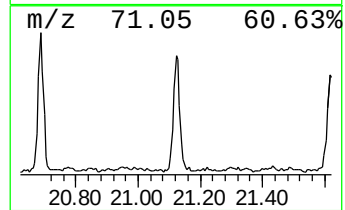
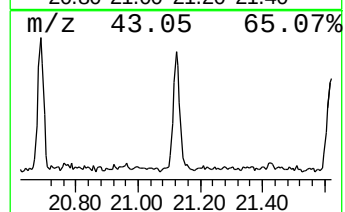
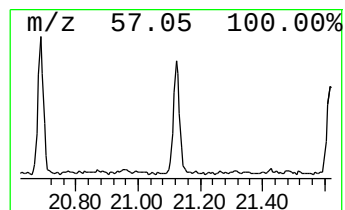
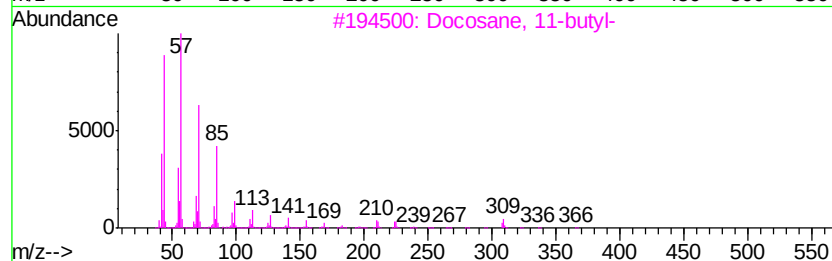
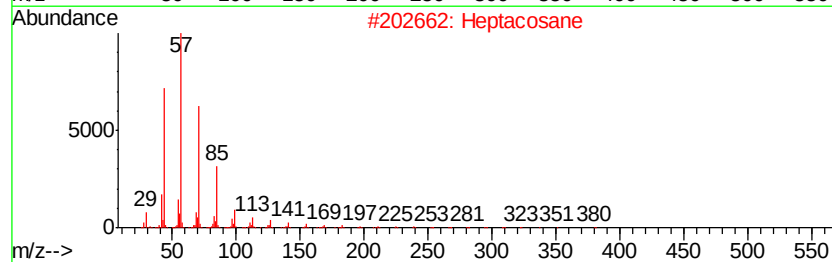
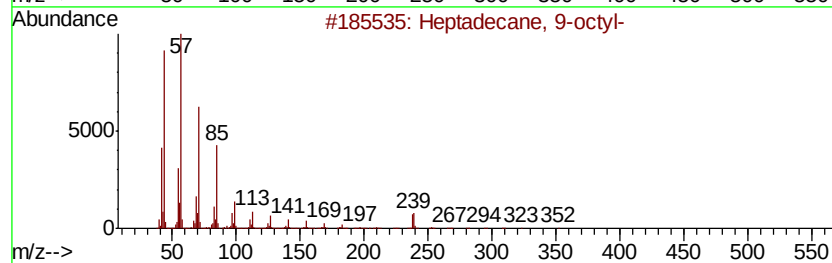
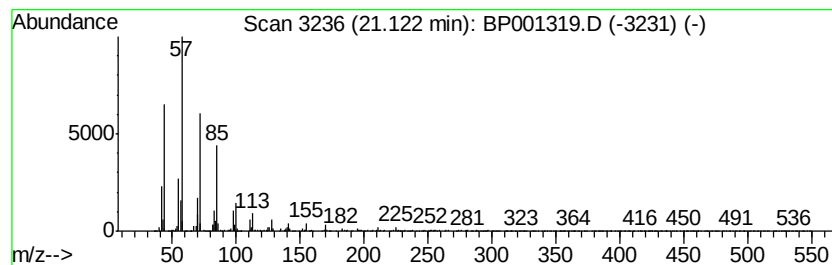
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecane, 9-octyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.12	3.56 ng	102056	Perylene-d12	21.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	98
2		Heptacosane	380	C27H56	000593-49-7	95
3		Docosane, 11-butyl-	366	C26H54	013475-76-8	94
4		Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	94
5		Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP121119\
Data File : BP001319.D
Acq On : 11 Dec 2019 18:58
Operator : JU
Sample : K6204-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K072-AB-WC-1

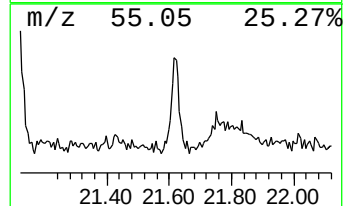
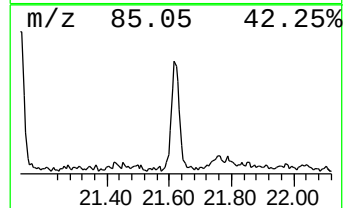
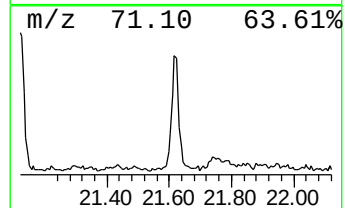
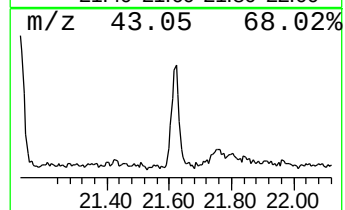
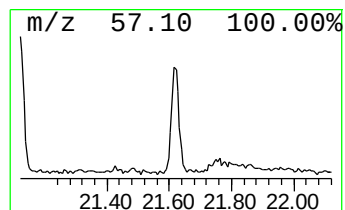
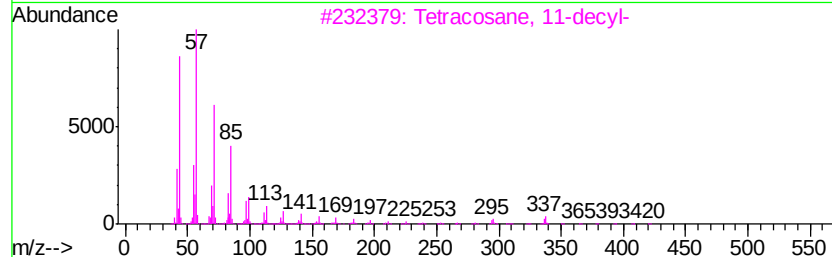
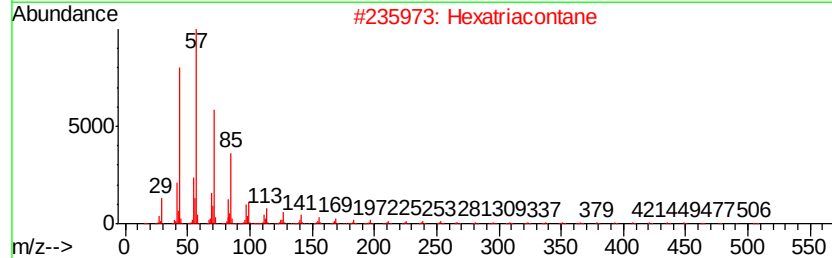
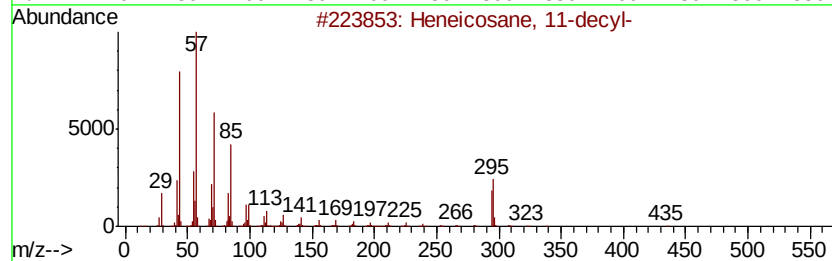
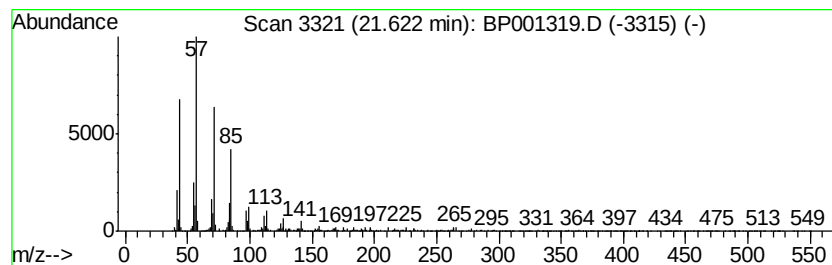
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane, 11-decyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.62	3.42 ng	98190	Perylene-d12	21.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	98
2		Hexatriacontane	507	C36H74	000630-06-8	97
3		Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
4		Heptadecane, 3-methyl-	254	C18H38	006418-44-6	90
5		Hentriacontane	437	C31H64	000630-04-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP121119\
Data File : BP001319.D
Acq On : 11 Dec 2019 18:58
Operator : JU
Sample : K6204-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
K072-AB-WC-1

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...	5.62	14.9	ng	358088	1	8.30	481160	20.0
unknown7.95	7.95	69.9	ng	1681220	1	8.30	481160	20.0
n-Hexadecanoic acid	16.49	2.2	ng	79646	4	15.60	712734	20.0
1-Heneicosanol	19.15	7.0	ng	238306	5	19.24	682588	20.0
Octadecane	20.29	2.8	ng	80160	6	21.01	573910	20.0
Docosane, 11-butyl-	20.69	3.4	ng	97249	6	21.01	573910	20.0
Heptadecane, 9-oc...	21.12	3.6	ng	102056	6	21.01	573910	20.0
Heneicosane, 11-d...	21.62	3.4	ng	98190	6	21.01	573910	20.0