

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
 Data File : BP001612.D
 Acq On : 15 Jan 2020 16:51
 Operator : JU
 Sample : L1126-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 BW-2-20.0

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-BP010820.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	2.870	10	14	23	rBV2	27316	48863	2.95%	0.474%
2	2.952	24	28	36	rVB	199448	226844	13.72%	2.201%
3	4.799	337	342	348	rBV	121464	163028	9.86%	1.582%
4	5.258	414	420	433	rBV	480854	723144	43.72%	7.015%
5	6.828	680	687	698	rBV	528033	844158	51.04%	8.189%
6	7.175	739	746	757	rBV	522195	801972	48.49%	7.780%
7	7.634	817	824	833	rBV	138017	213048	12.88%	2.067%
8	7.952	871	878	888	rVB	403272	632639	38.25%	6.137%
9	8.781	1011	1019	1039	rBV	317185	537956	32.53%	5.219%
10	10.410	1287	1296	1309	rBV	147135	261336	15.80%	2.535%
11	12.898	1710	1719	1732	rBV	734612	1080046	65.30%	10.477%
12	13.746	1856	1863	1874	rBV	26110	46754	2.83%	0.454%
13	14.281	1947	1954	1971	rBV	239617	347302	21.00%	3.369%
14	15.781	2203	2209	2232	rBV	610292	876016	52.97%	8.498%
15	17.045	2417	2424	2433	rBV	278477	423519	25.61%	4.108%
16	17.975	2578	2582	2591	rBV2	30170	48715	2.95%	0.473%
17	19.633	2858	2864	2882	rBV	1370922	1653919	100.00%	16.044%
18	20.898	3074	3079	3093	rBV	91501	168764	10.20%	1.637%
19	21.145	3116	3121	3131	rBV	342168	470469	28.45%	4.564%
20	21.769	3224	3227	3231	rBV4	13218	20422	1.23%	0.198%
21	22.239	3304	3307	3312	rVB2	23354	31474	1.90%	0.305%
22	22.369	3325	3329	3334	rVB	66356	85799	5.19%	0.832%
23	22.751	3390	3394	3399	rBV	38090	53325	3.22%	0.517%
24	23.327	3489	3492	3495	rBV	35202	53371	3.23%	0.518%
25	23.380	3495	3501	3512	rVB	220665	432486	26.15%	4.195%
26	23.992	3601	3605	3611	rVB2	35689	63050	3.81%	0.612%

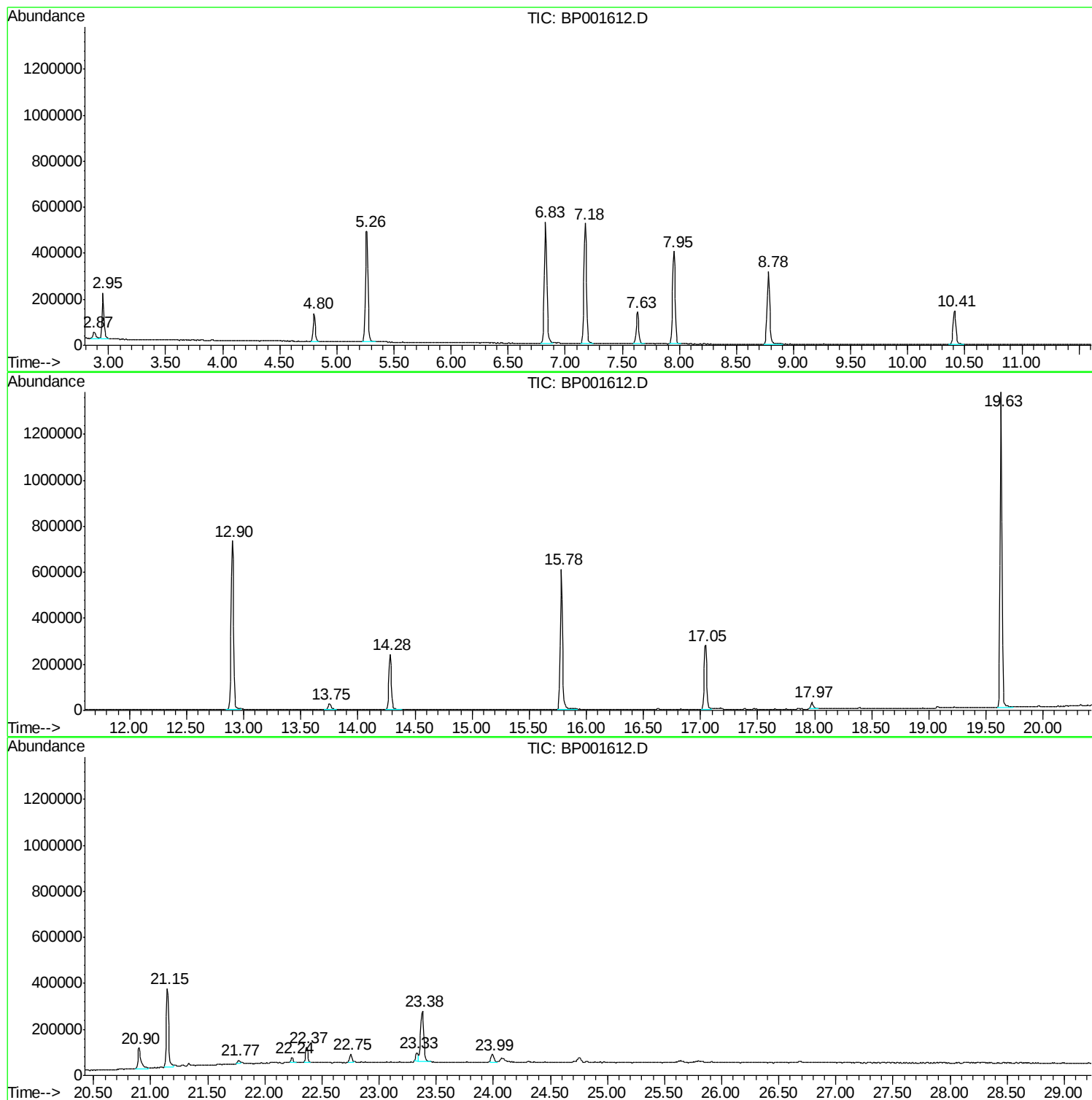
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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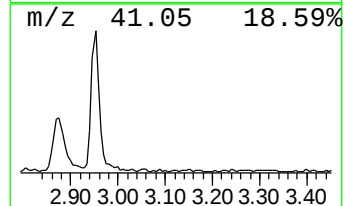
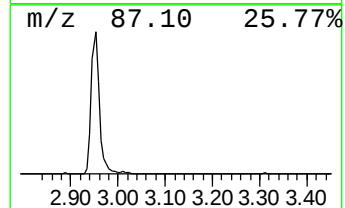
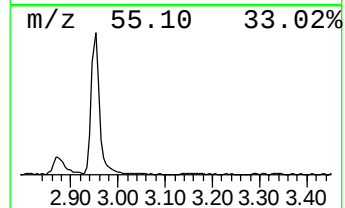
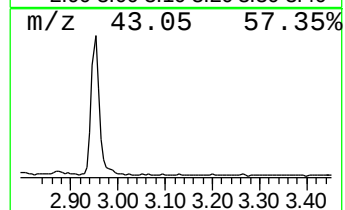
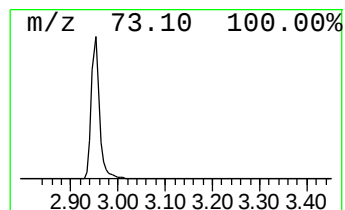
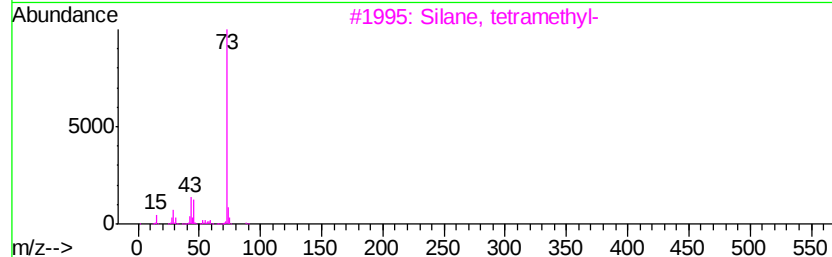
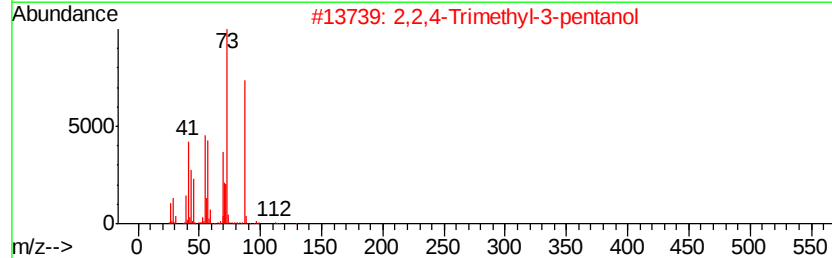
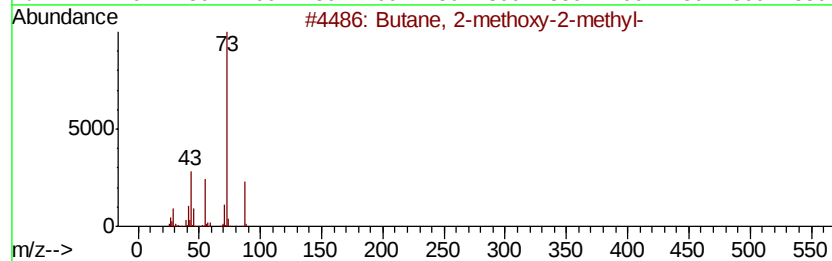
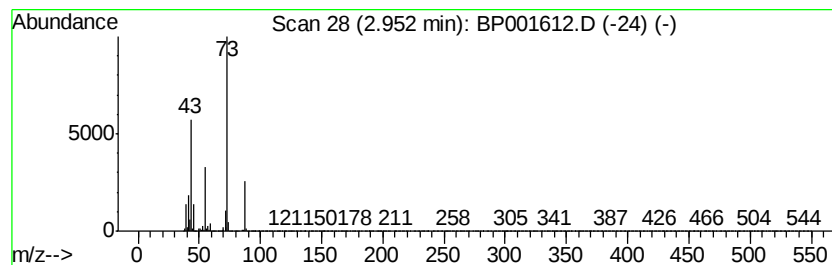
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.95	21.30 ng	226844	1,4-Dichlorobenzene-d4	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		4-Penten-2-ol, acetate	128	C7H12O2	1000352-31-5	10
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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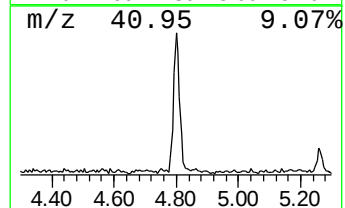
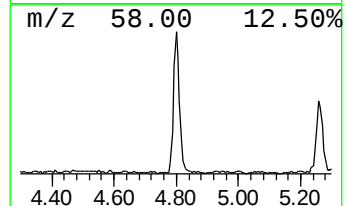
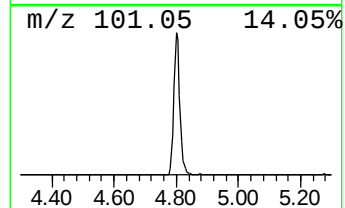
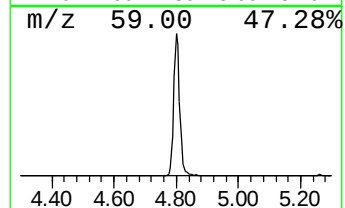
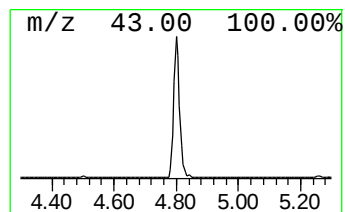
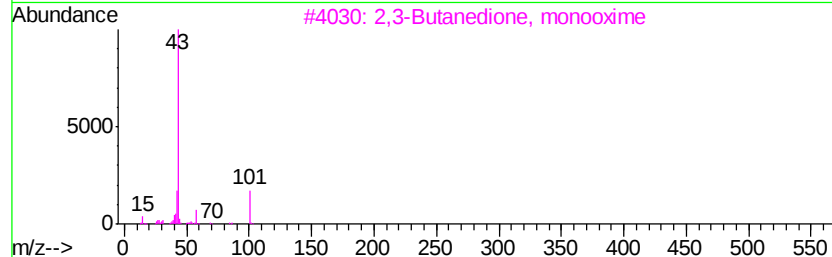
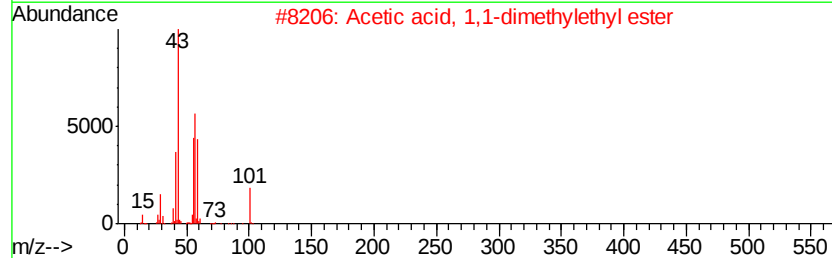
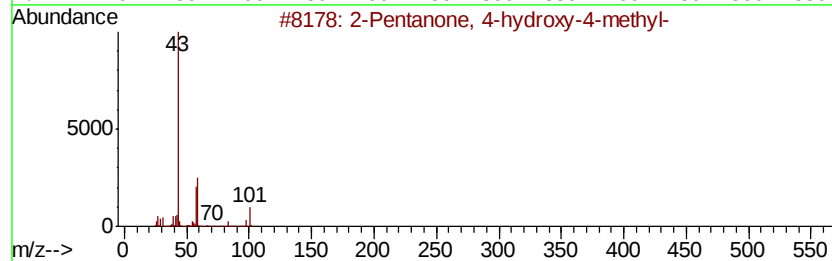
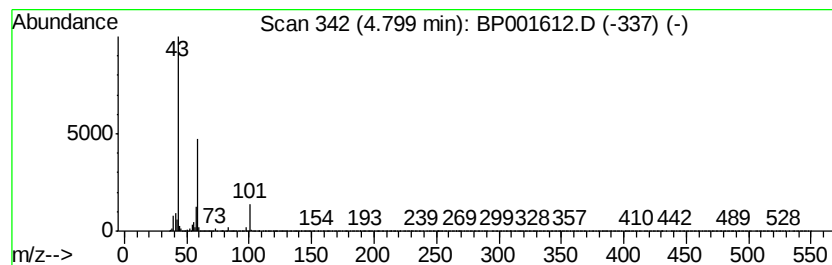
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	15.30 ng	163028	1,4-Dichlorobenzene-d4	7.63

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	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		Butane	58	C4H10	000106-97-8	9
5		1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	9



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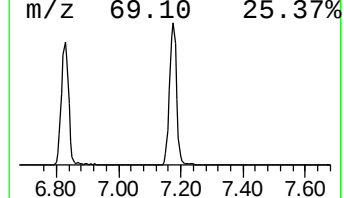
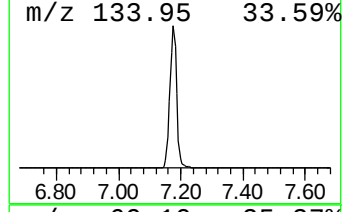
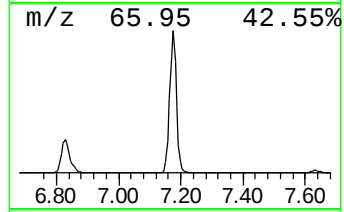
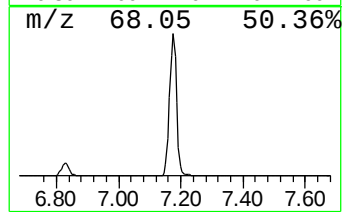
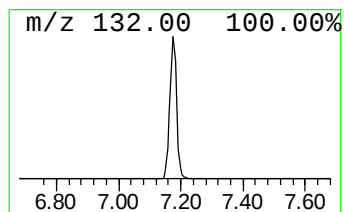
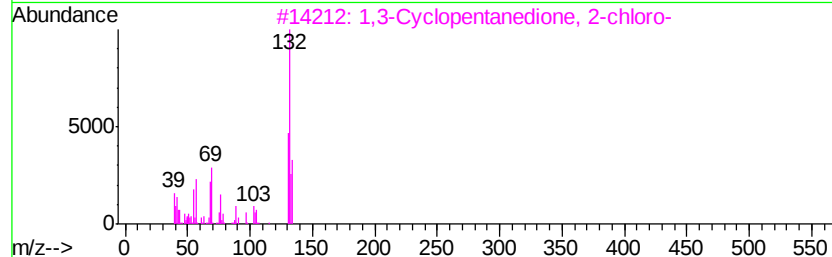
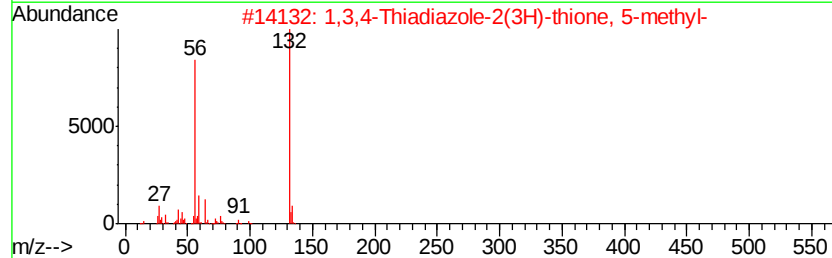
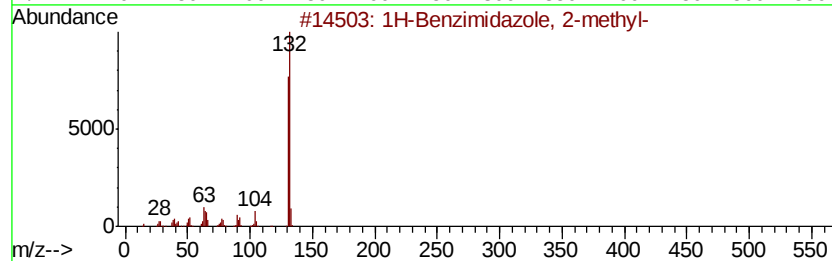
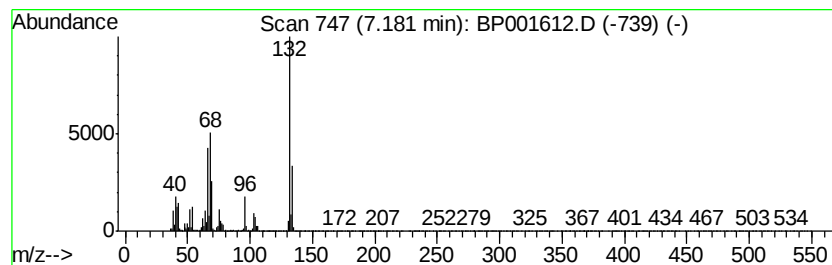
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown7.18 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	75.29 ng	801972	1,4-Dichlorobenzene-d4	7.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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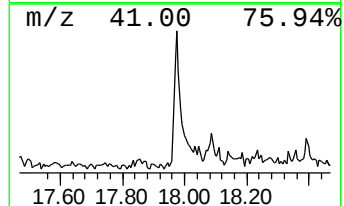
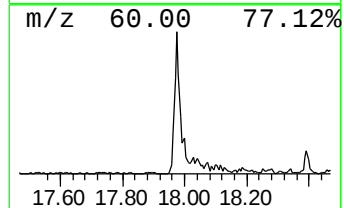
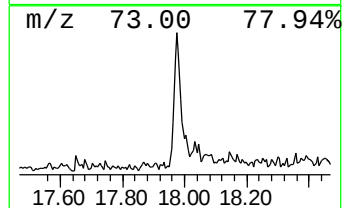
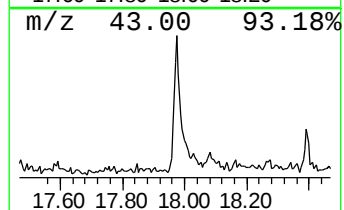
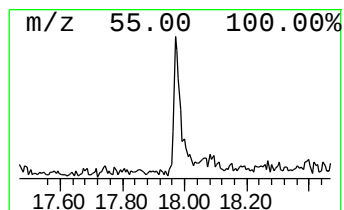
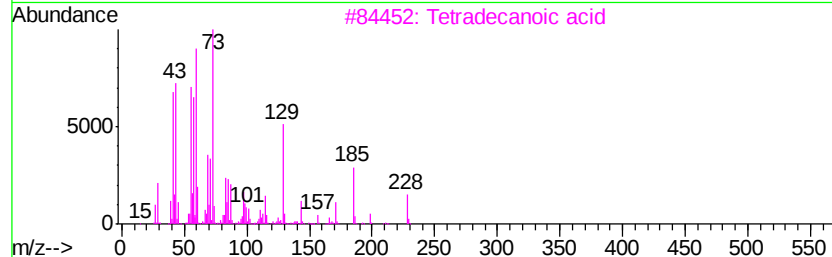
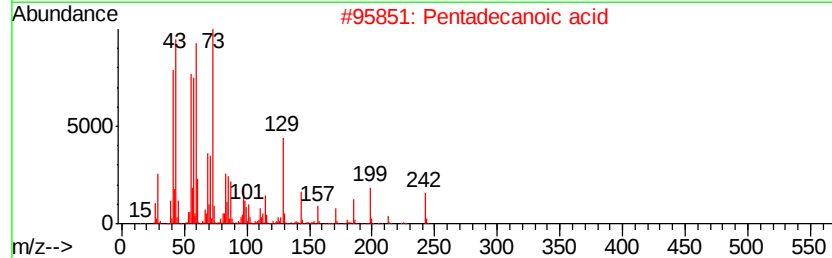
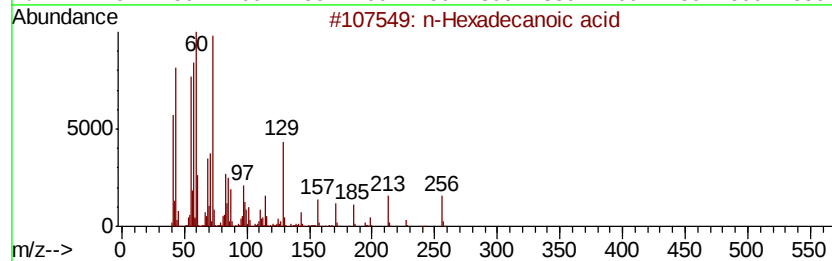
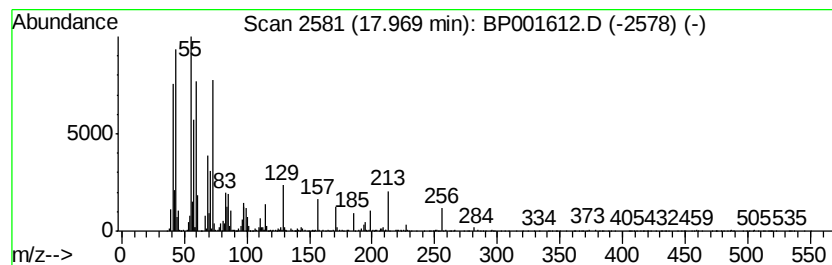
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.97	2.30 ng	48715	Phenanthrene-d10	17.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		n-Decanoic acid	172	C10H20O2	000334-48-5	53



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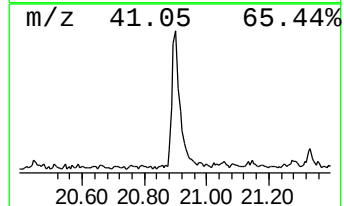
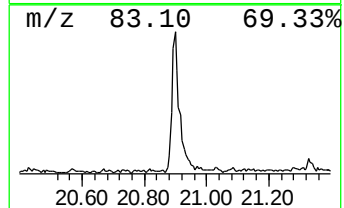
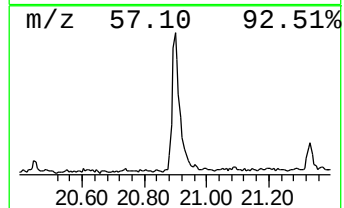
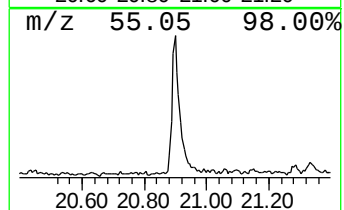
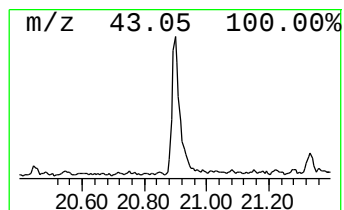
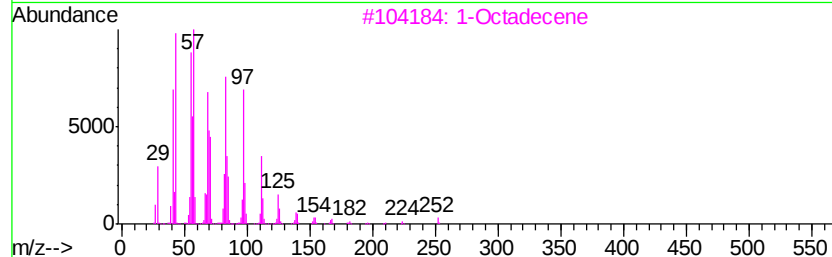
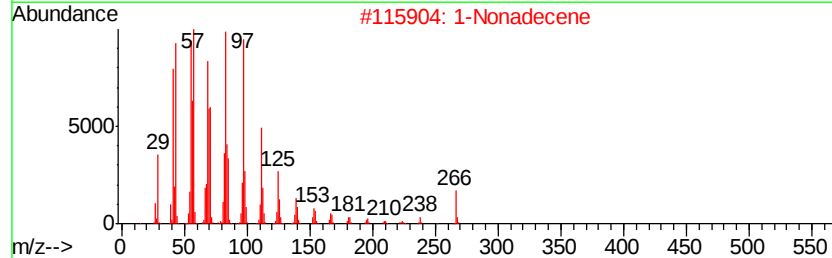
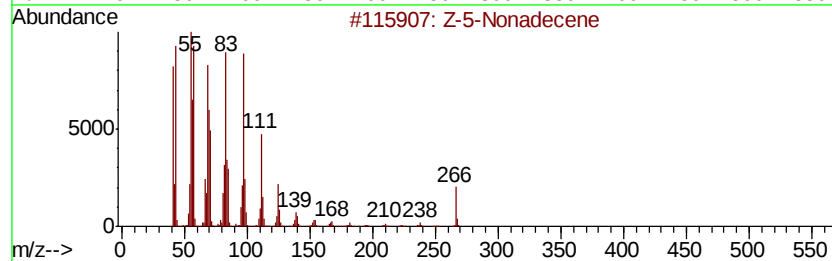
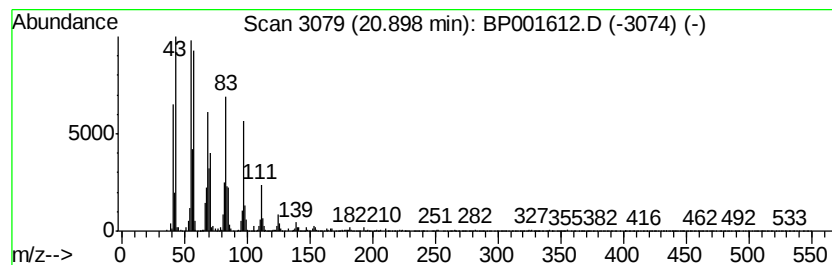
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Z-5-Nonadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	7.17 ng	168764	Chrysene-d12	21.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Z-5-Nonadecene	266	C19H38	1000131-11-8	95
2		1-Nonadecene	266	C19H38	018435-45-5	95
3		1-Octadecene	252	C18H36	000112-88-9	95
4		Cyclopentadecane	210	C15H30	000295-48-7	95
5		Cyclotetracosane	336	C24H48	000297-03-0	94



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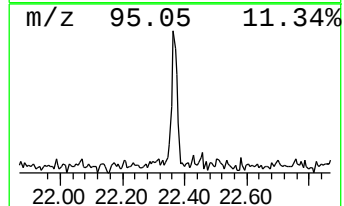
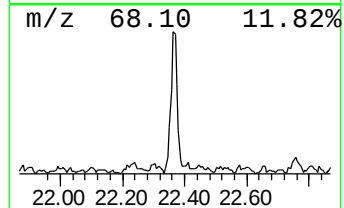
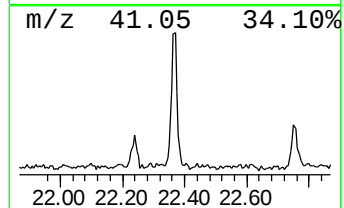
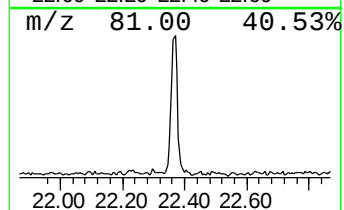
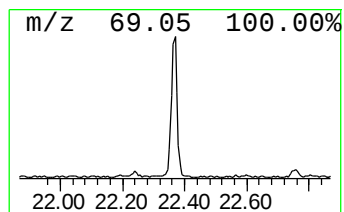
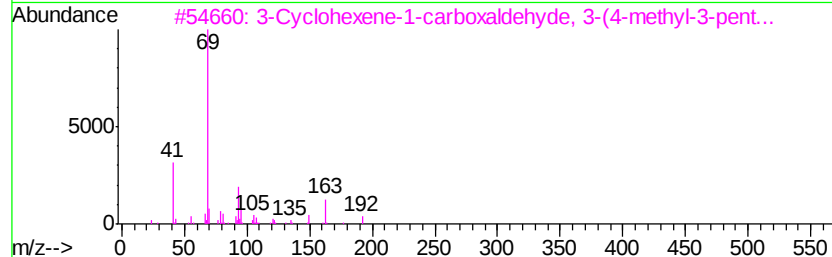
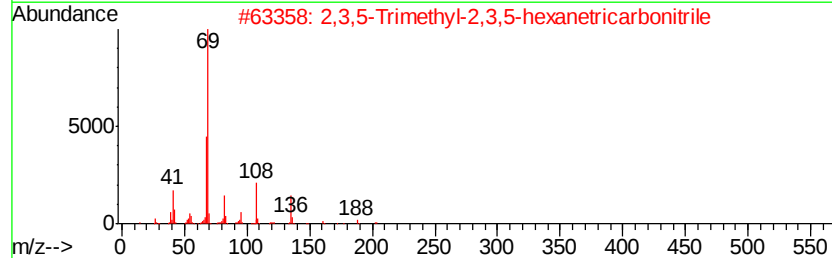
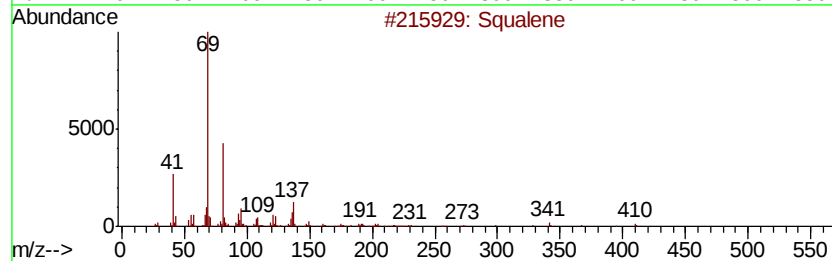
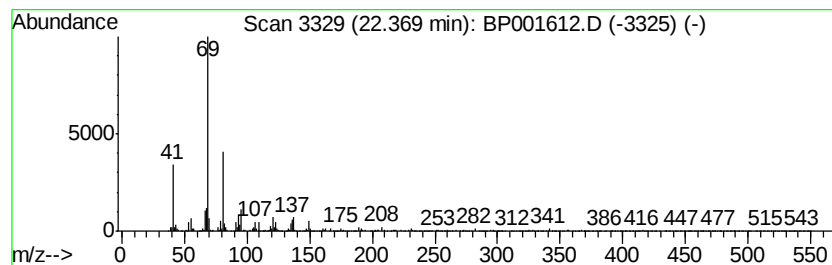
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	3.97 ng	85799	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	72
2		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	72
3		3-Cyclohexene-1-carboxaldehyde, ...	192	C13H20O	052475-89-5	64
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5		trans-Geranylgeraniol	290	C20H34O	024034-73-9	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001612.D
Acq On : 15 Jan 2020 16:51
Operator : JU
Sample : L1126-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BW-2-20.0

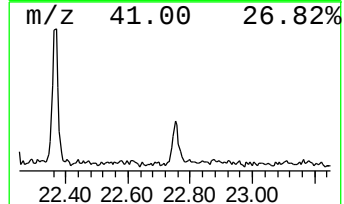
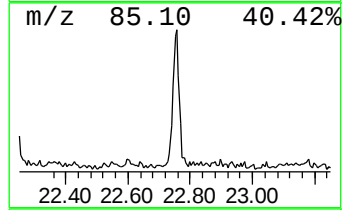
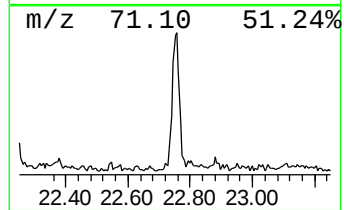
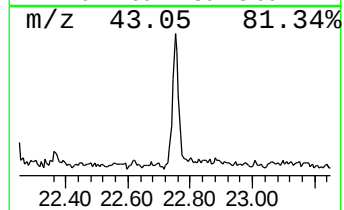
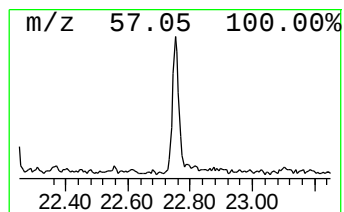
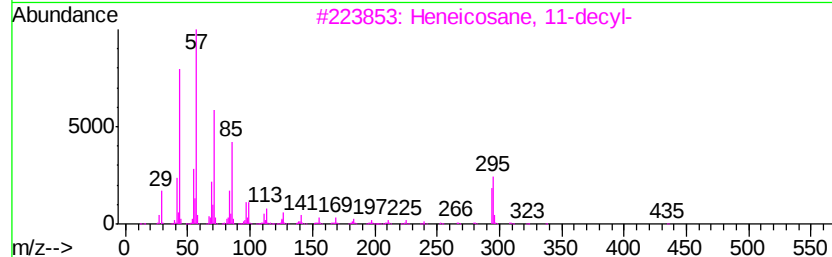
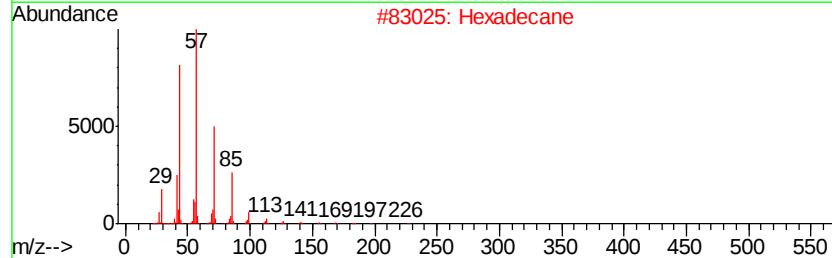
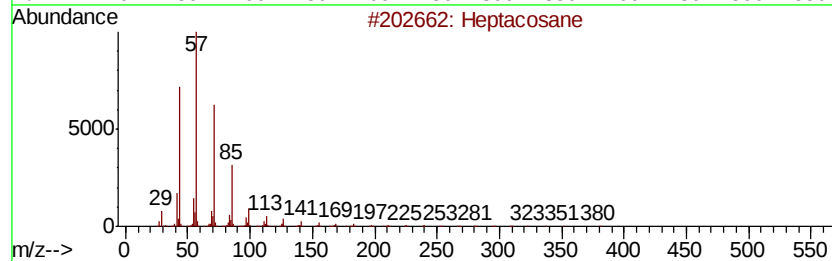
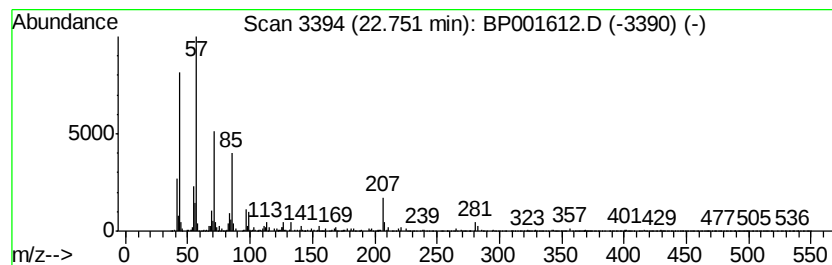
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.75	2.47 ng	53325	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	96
2		Hexadecane	226	C16H34	000544-76-3	90
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	81
4		Behenyl chloride	344	C22H45Cl	042217-03-8	81
5		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001612.D
Acq On : 15 Jan 2020 16:51
Operator : JU
Sample : L1126-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BW-2-20.0

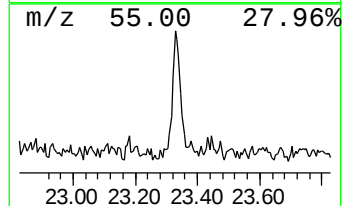
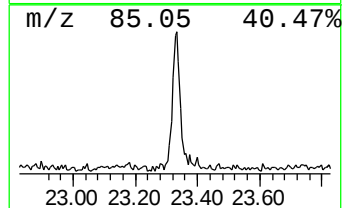
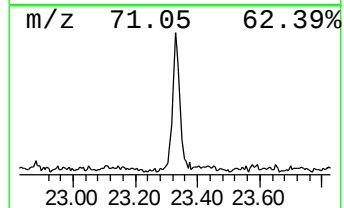
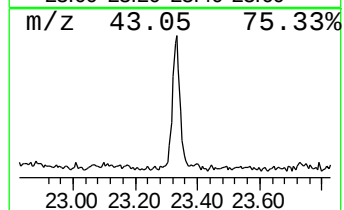
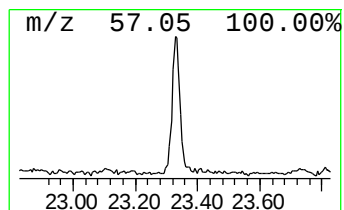
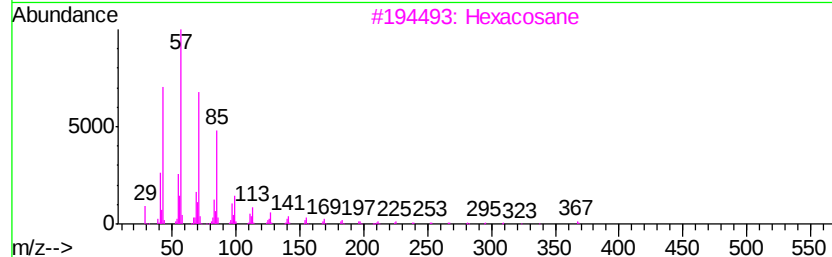
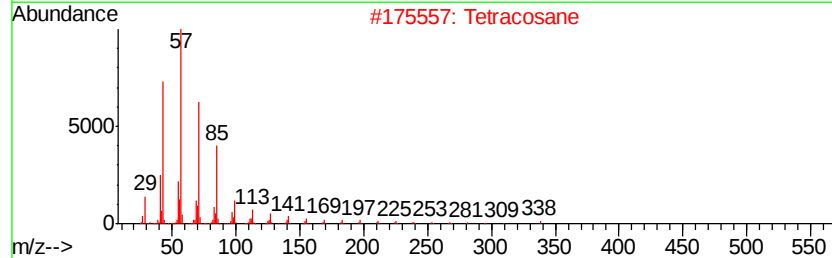
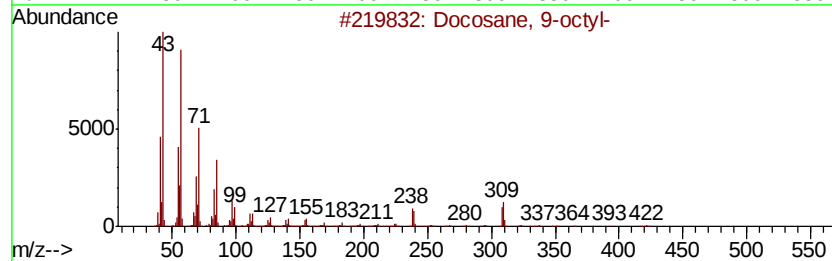
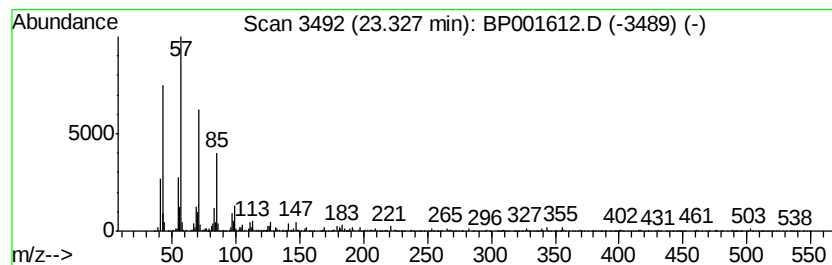
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.33	2.47 ng	53371	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane, 9-octyl-	422	C30H62	055319-83-0	89
2		Tetracosane	338	C24H50	000646-31-1	87
3		Hexacosane	366	C26H54	000630-01-3	87
4		Octacosane	394	C28H58	000630-02-4	83
5		Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP011520\
Data File : BP001612.D
Acq On : 15 Jan 2020 16:51
Operator : JU
Sample : L1126-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BW-2-20.0

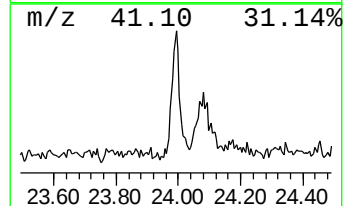
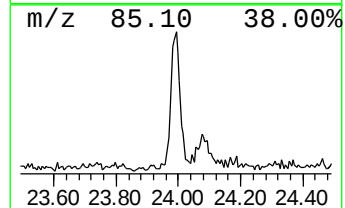
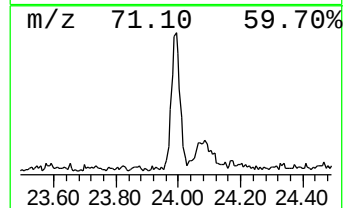
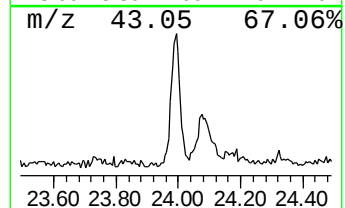
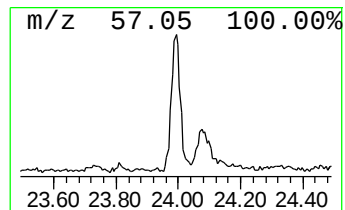
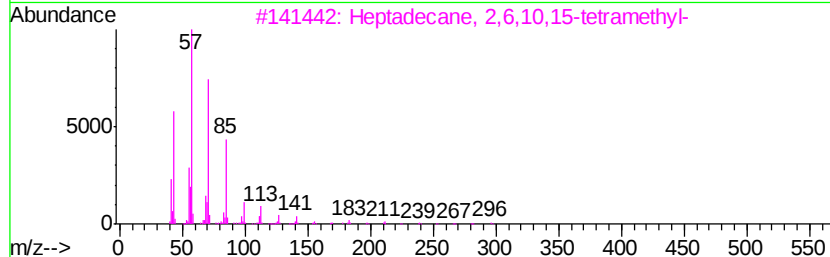
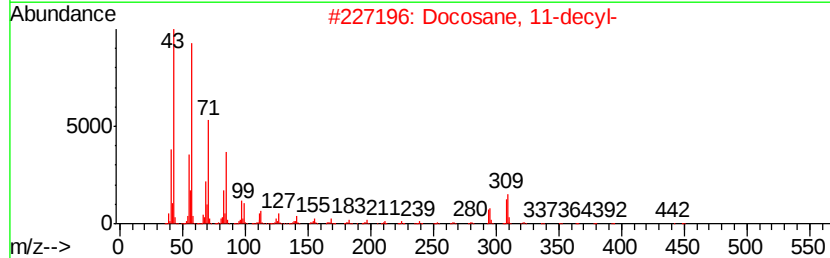
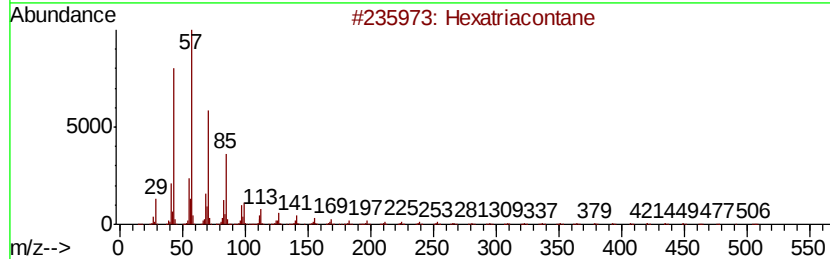
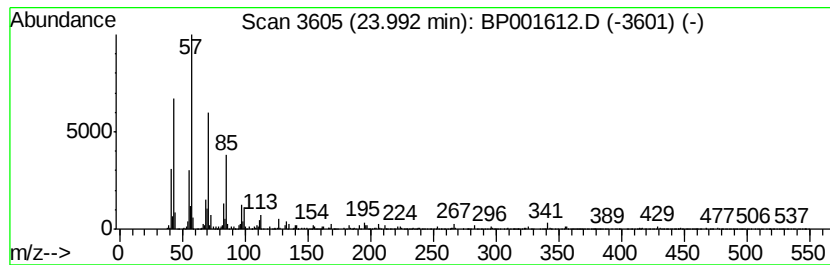
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Hexatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	2.92 ng	63050	Perylene-d12	23.38

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexatriacontane	507	C36H74	000630-06-8	93
2		Docosane, 11-decyl-	451	C32H66	055401-55-3	91
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
4		Tricosane	324	C23H48	000638-67-5	87
5		Tricosane, 2-methyl-	338	C24H50	001928-30-9	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP011520\
Data File : BP001612.D
Acq On : 15 Jan 2020 16:51
Operator : JU
Sample : L1126-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
BW-2-20.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP010820.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
Butane, 2-methoxy...	2.95	21.3	ng	226844	1	7.63	213048	20.0
2-Pentanone, 4-hy...	4.80	15.3	ng	163028	1	7.63	213048	20.0
unknown7.18	7.18	75.3	ng	801972	1	7.63	213048	20.0
n-Hexadecanoic acid	17.97	2.3	ng	48715	4	17.05	423519	20.0
Z-5-Nonadecene	20.90	7.2	ng	168764	5	21.15	470469	20.0
Squalene	22.37	4.0	ng	85799	6	23.38	432486	20.0
Heptacosane	22.75	2.5	ng	53325	6	23.38	432486	20.0
Docosane, 9-octyl-	23.33	2.5	ng	53371	6	23.38	432486	20.0
Hexatriacontane	23.99	2.9	ng	63050	6	23.38	432486	20.0