

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040521\
 Data File : BP005178.D
 Acq On : 05 Apr 2021 14:49
 Operator : CG/JU
 Sample : M1897-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-2

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\8270E-BP032321.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005178.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.299	369	376	385	rBV	636810	882755	47.32%	8.821%
2	6.887	636	646	657	rBV	561211	914872	49.04%	9.142%
3	7.705	777	785	791	rBV	100562	161677	8.67%	1.615%
4	8.863	973	982	990	rBV	349680	580254	31.10%	5.798%
5	10.493	1252	1259	1266	rBV	131827	216429	11.60%	2.163%
6	12.975	1672	1681	1690	rBV	842876	1253762	67.20%	12.528%
7	13.128	1702	1707	1710	rBV4	26604	43734	2.34%	0.437%
8	13.769	1812	1816	1820	rBV	52100	77411	4.15%	0.774%
9	13.893	1834	1837	1845	rVB5	37390	74413	3.99%	0.744%
10	14.004	1853	1856	1860	rBV5	28764	36557	1.96%	0.365%
11	14.098	1867	1872	1878	rBV6	69564	185176	9.93%	1.850%
12	14.187	1883	1887	1894	rVB	172757	270883	14.52%	2.707%
13	14.322	1906	1910	1912	rBV3	82681	120348	6.45%	1.203%
14	14.357	1913	1916	1924	rVB	215607	327100	17.53%	3.268%
15	14.887	2003	2006	2012	rBV6	70648	138235	7.41%	1.381%
16	15.151	2047	2051	2056	rBV2	226404	294829	15.80%	2.946%
17	15.863	2167	2172	2177	rBV	584668	845954	45.34%	8.453%
18	17.128	2383	2387	2394	rBV	275123	471181	25.26%	4.708%
19	18.028	2537	2540	2544	rBV	239282	319778	17.14%	3.195%
20	19.704	2820	2825	2833	rVB	1455281	1865619	100.00%	18.642%
21	20.933	3031	3034	3042	rVB2	150362	211845	11.36%	2.117%
22	21.222	3079	3083	3087	rVB	295725	350339	18.78%	3.501%
23	23.504	3466	3471	3480	rVB2	191509	364721	19.55%	3.644%

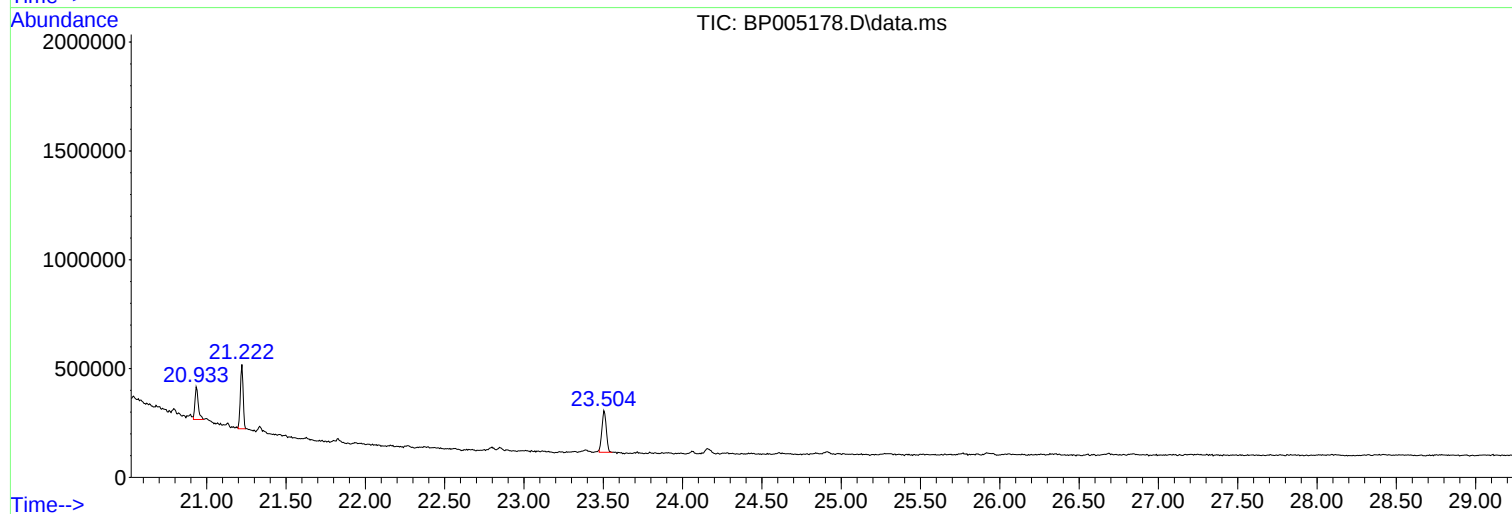
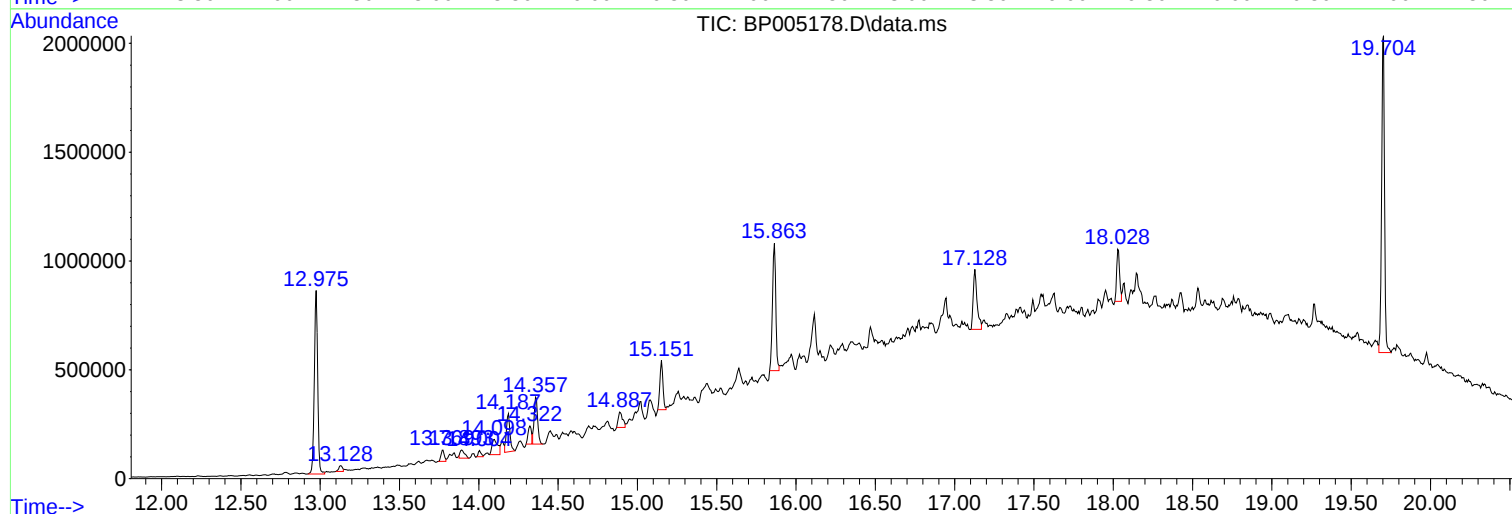
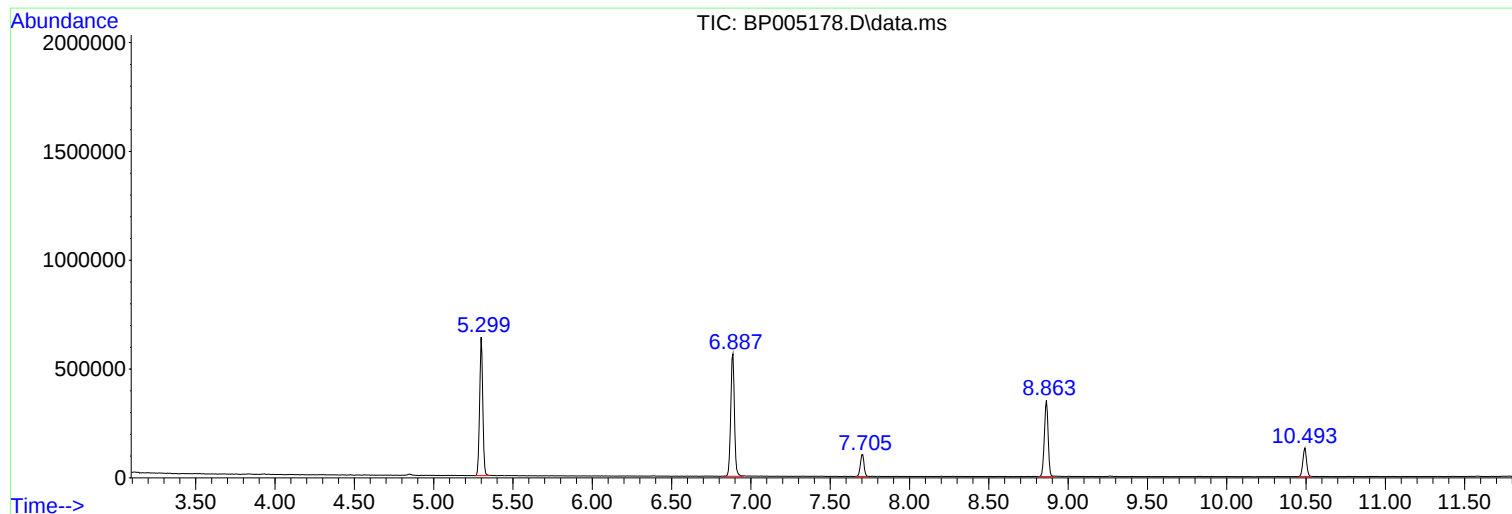
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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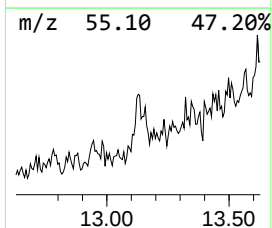
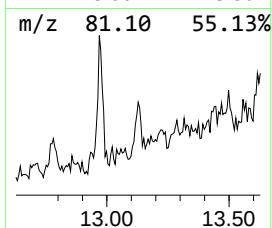
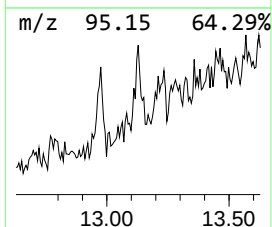
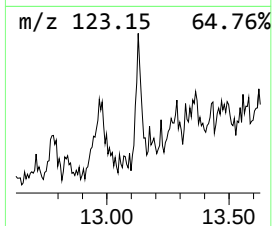
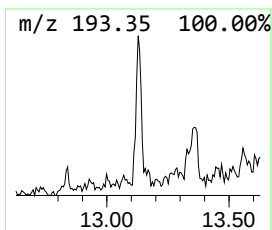
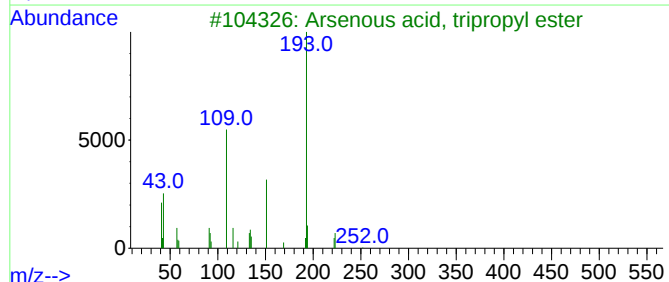
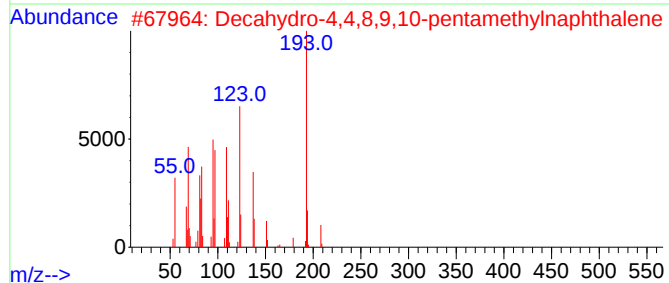
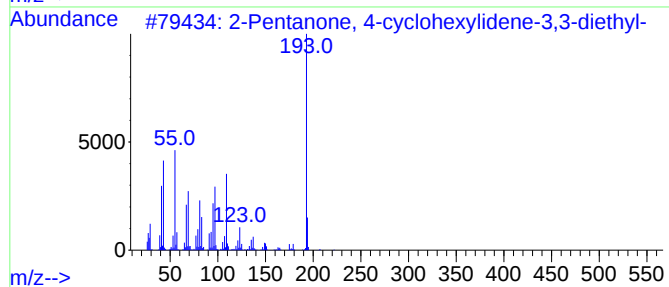
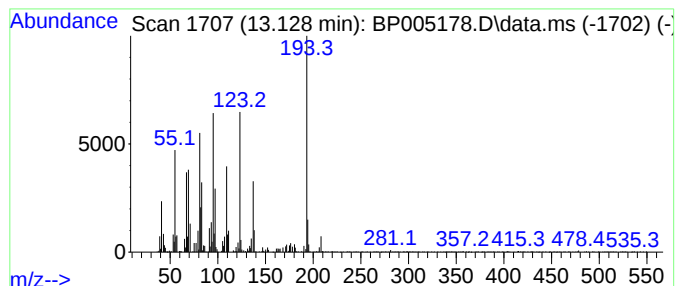
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-cyclohexylidene-3... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	2.67 ng	43734	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	92		
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	52		
3	Arsenous acid, tripropyl ester	252	C9H21AsO3	015606-91-4	43		
4	6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	38		
5	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	37		



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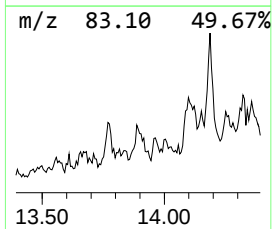
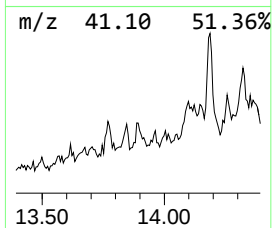
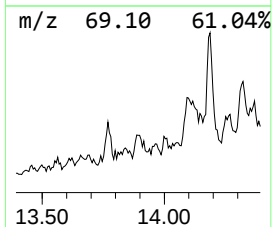
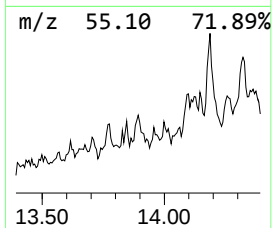
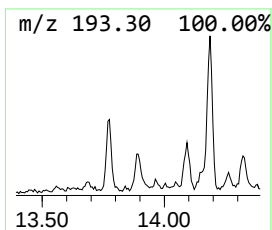
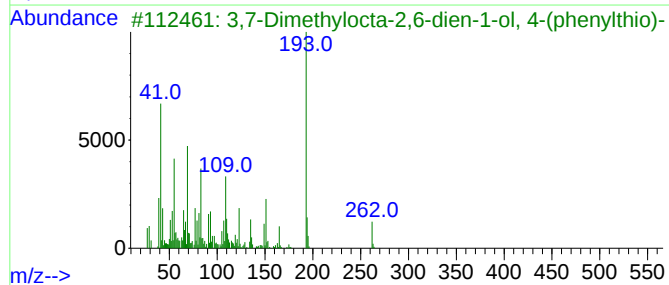
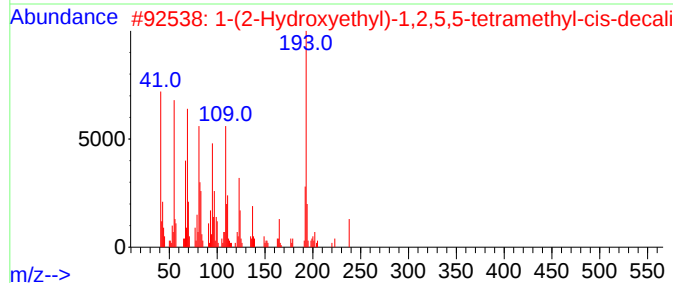
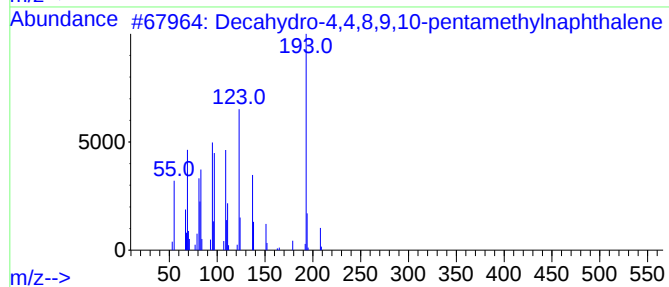
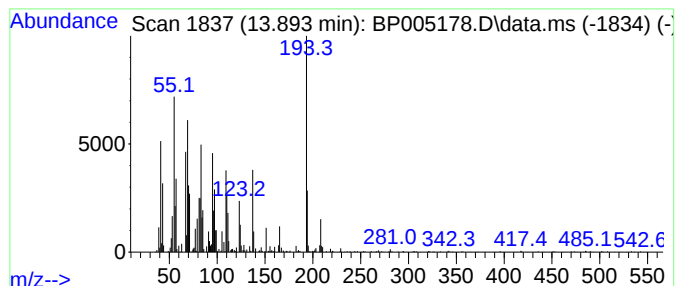
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Decahydro-4,4,8,9,10-pentam... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.893	4.55 ng	74413	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	74
2			1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	64
3			3,7-Dimethylocta-2,6-dien-1-ol, ...	262	C16H22OS	1000196-46-7	32
4			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	25
5			2-Aminophenanthrene	193	C14H11N	003366-65-2	25



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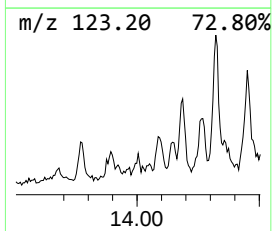
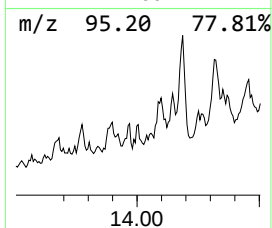
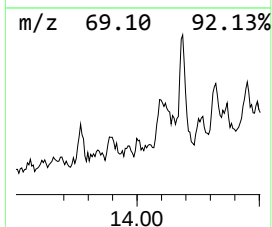
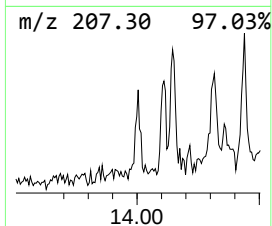
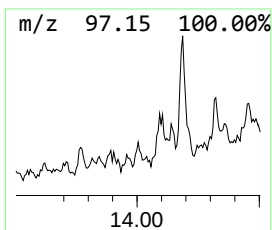
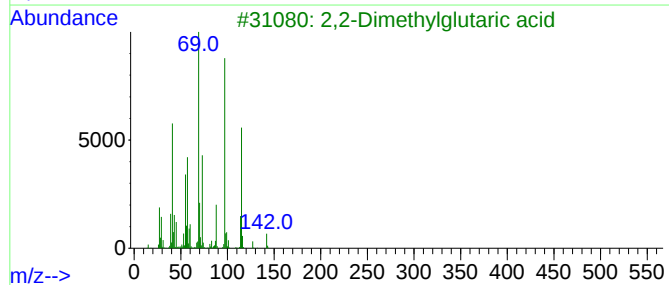
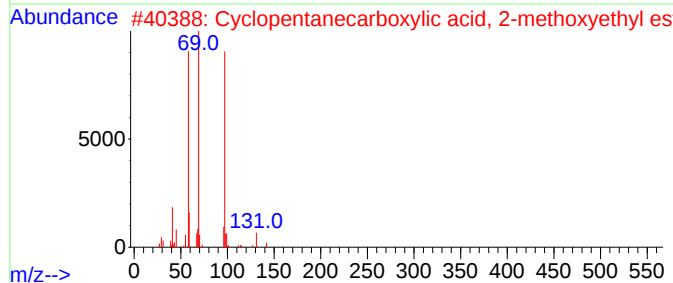
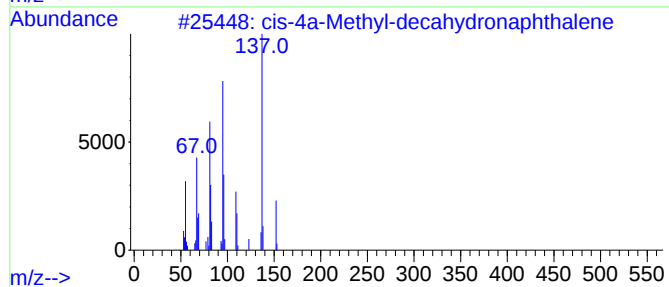
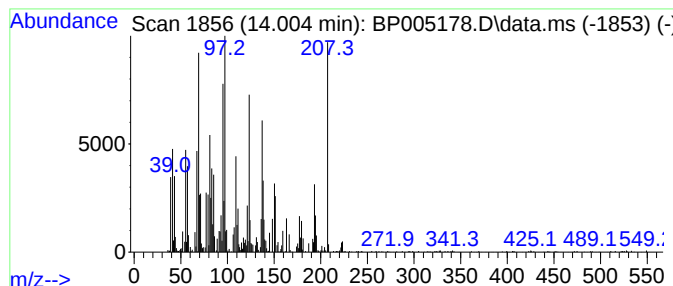
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.00 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	2.24 ng	36557	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-4a-Methyl-decahydronaphthalene	152	C11H20	002547-26-4	14
2			Cyclopentanecarboxylic acid, 2-m...	172	C9H16O3	1000331-06-9	14
3			2,2-Dimethylglutaric acid	160	C7H12O4	000681-57-2	14
4			1-Propanone, 1-[2-methyl-5-(1-me...	194	C13H22O	031375-17-4	14
5			1-Butyne, 3-ethoxy-3-methyl-	112	C7H12O	007740-69-4	14



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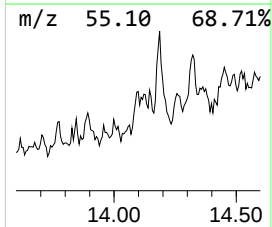
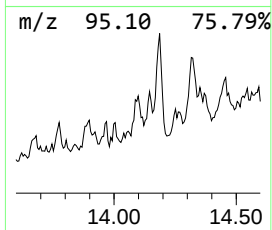
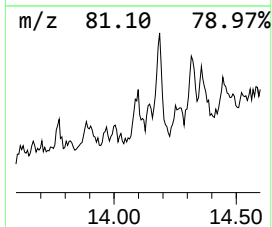
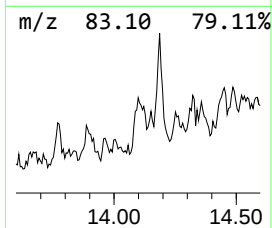
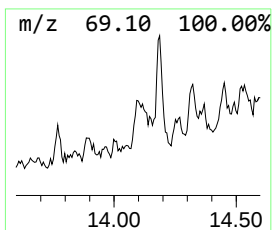
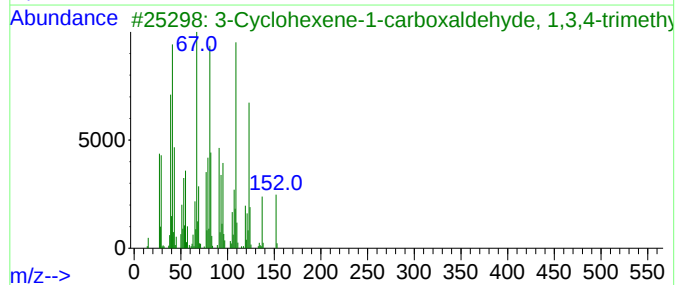
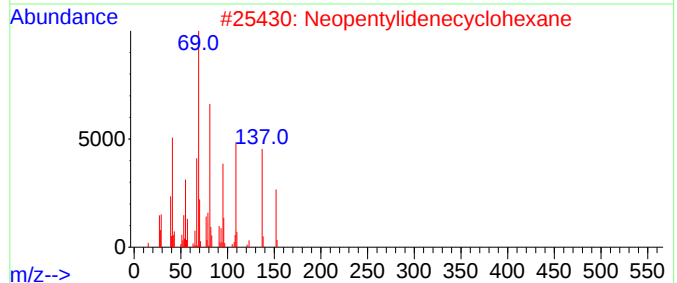
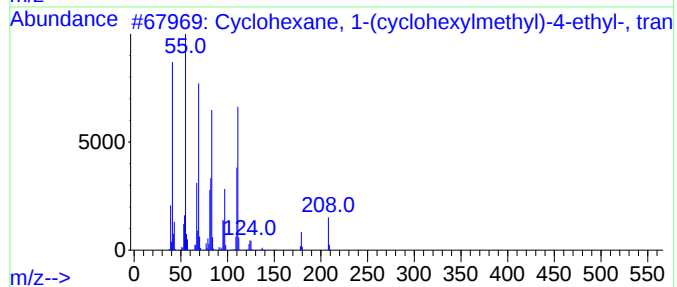
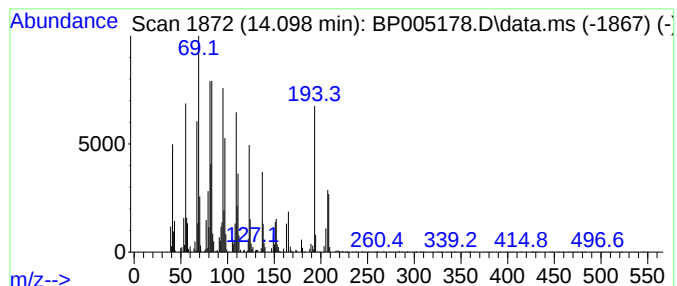
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.09 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	11.32 ng	185176	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-(cyclohexylmethyl)...	208	C15H28	054934-94-0	38
2			Neopentylidenecyclohexane	152	C11H20	039546-80-0	38
3			3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	040702-26-9	38
4			2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	30
5			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	25



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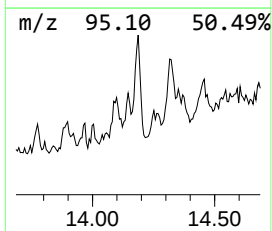
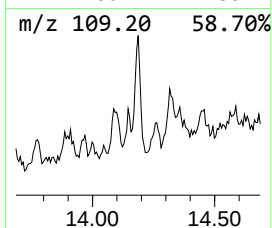
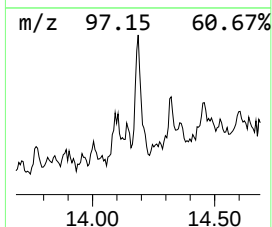
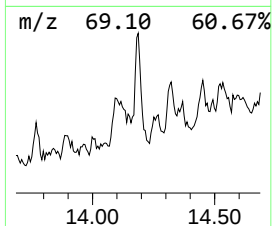
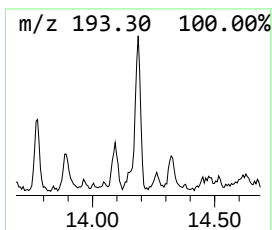
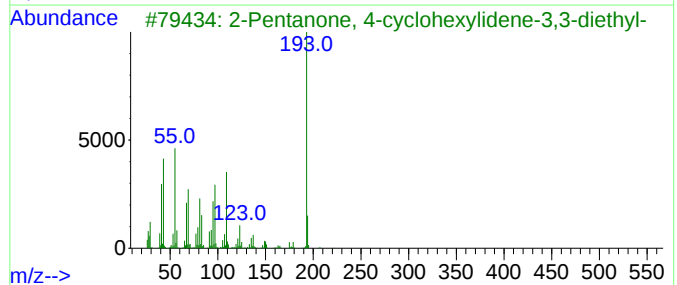
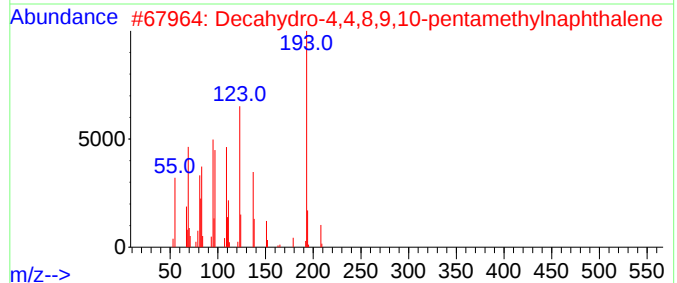
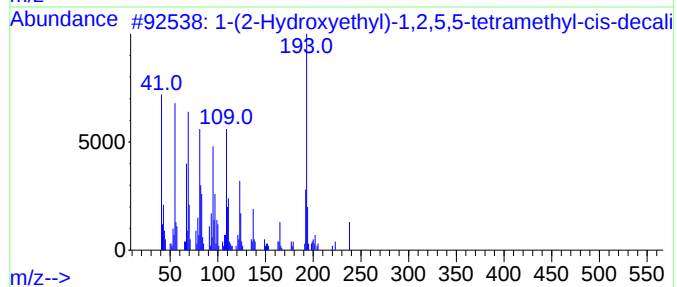
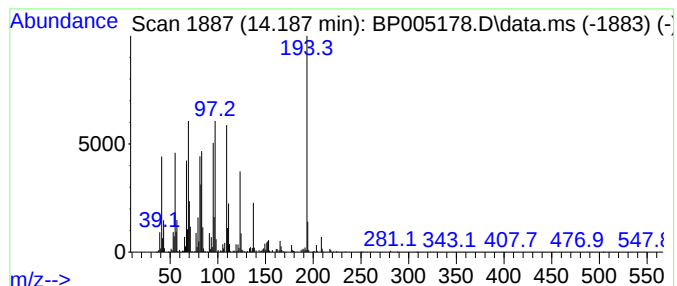
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-(2-Hydroxyethyl)-1,2,5,5-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.187	16.56 ng	270883	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Hydroxyethyl)-1,2,5,5-tetra...	238	C16H30O	1000298-97-4	72		
2	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	43		
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	42		
4	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1000162-56-0	35		
5	2-Diethylamino-4-phenylthiooct-2...	302	C18H26N2S	1000090-57-0	35		



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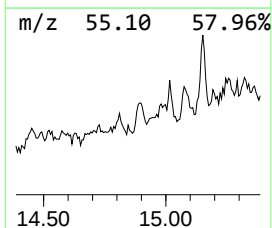
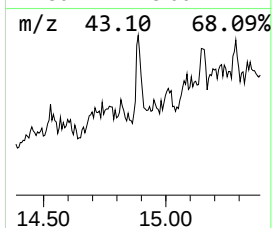
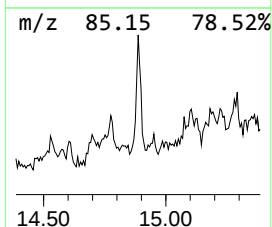
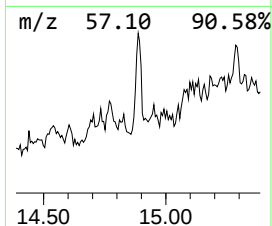
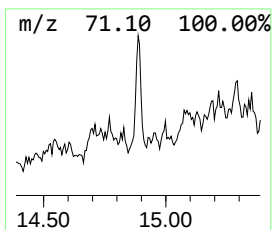
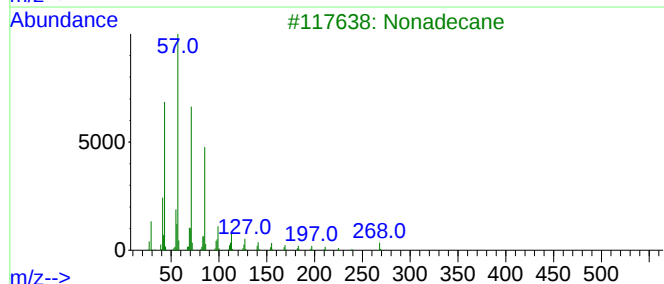
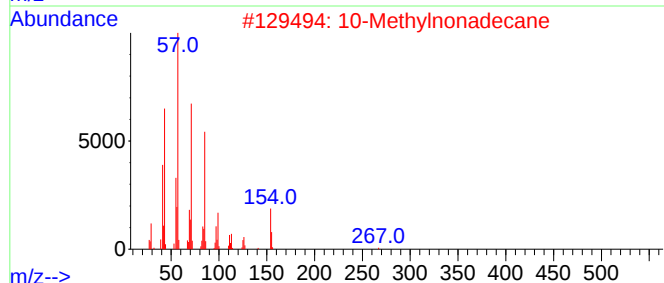
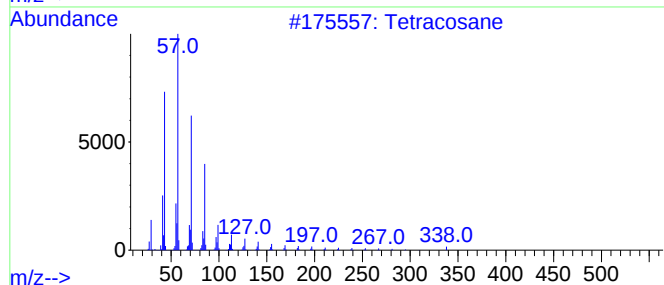
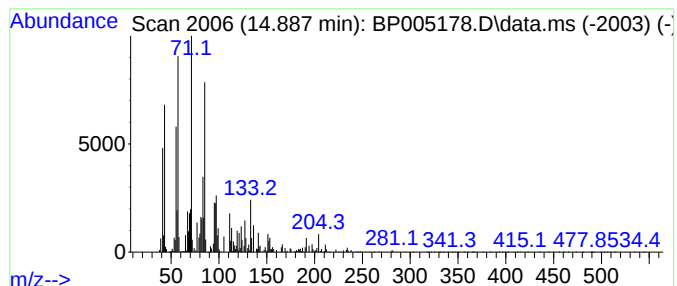
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.887	8.45 ng	138235	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	52
2			10-Methylnonadecane	282	C20H42	056862-62-5	49
3			Nonadecane	268	C19H40	000629-92-5	49
4			Decane, 3-methyl-	156	C11H24	013151-34-3	49
5			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040521\
Data File : BP005178.D
Acq On : 05 Apr 2021 14:49
Operator : CG/JU
Sample : M1897-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

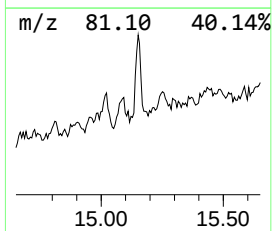
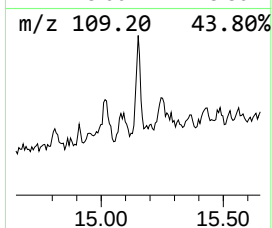
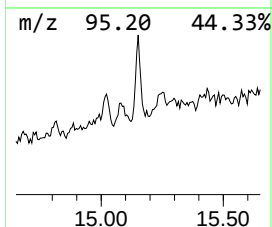
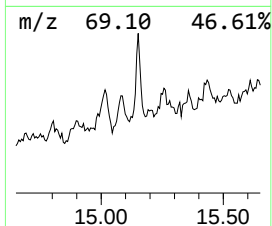
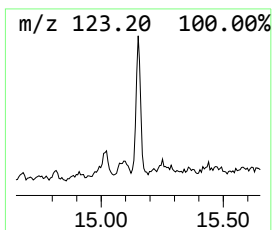
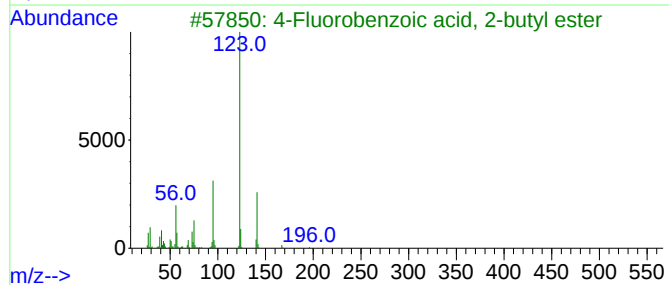
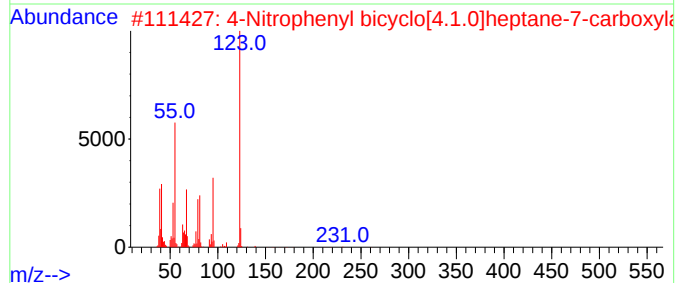
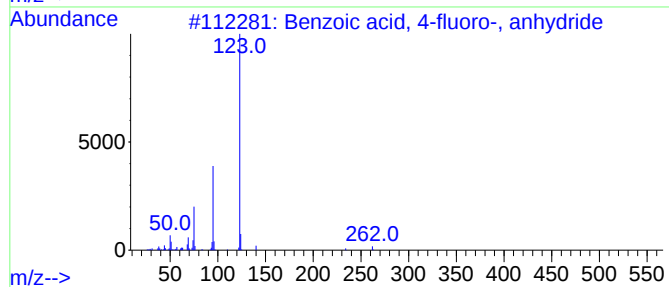
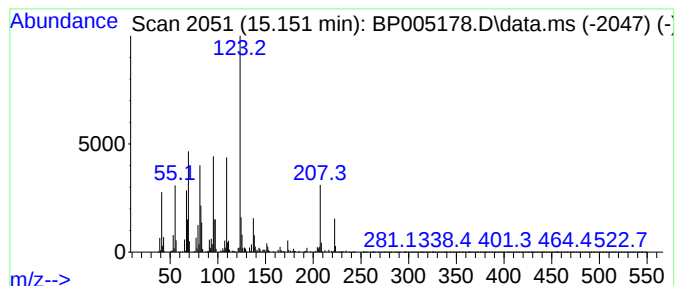
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.15 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.151	18.03 ng	294829	Acenaphthene-d10	14.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 4-fluoro-, anhydride	262	C14H8F2O3	025569-77-1	43
2			4-Nitrophenyl bicyclo[4.1.0]hept...	261	C14H15NO4	328938-65-4	43
3			4-Fluorobenzoic acid, 2-butyl ester	196	C11H13FO2	090172-12-6	43
4			3-Fluorobenzoic acid, 4-cyanophe...	241	C14H8FN02	1000307-72-8	43
5			3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040521\
Data File : BP005178.D
Acq On : 05 Apr 2021 14:49
Operator : CG/JU
Sample : M1897-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

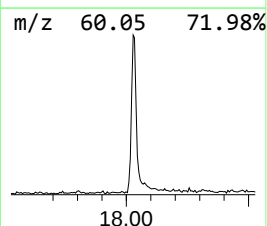
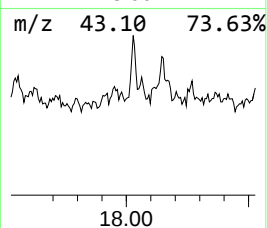
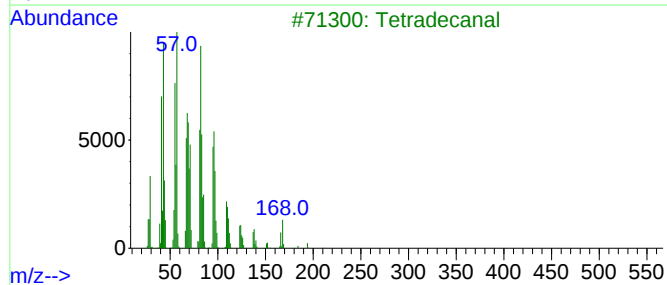
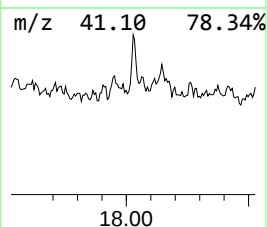
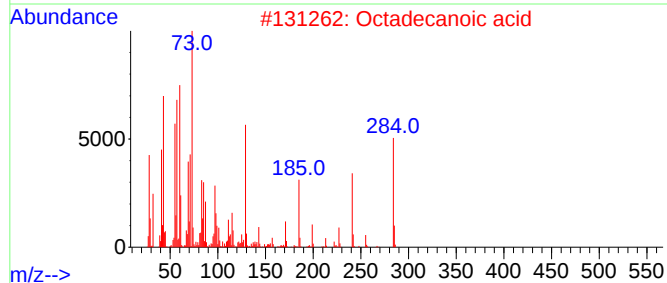
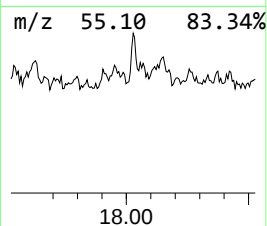
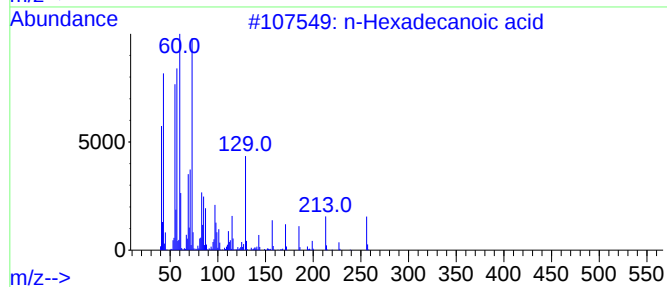
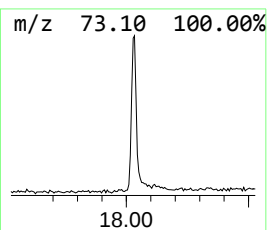
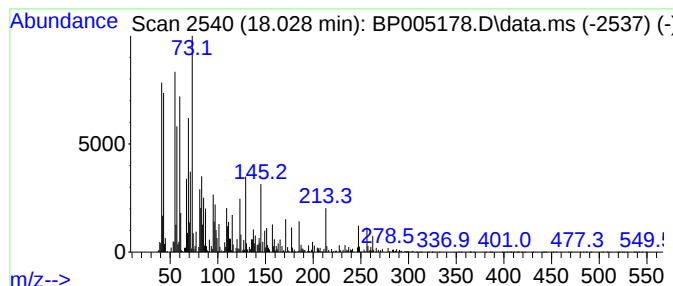
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.028	13.57 ng	319778	Phenanthrene-d10	17.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Octadecanoic acid	284	C18H36O2	000057-11-4	46
3			Tetradecanal	212	C14H28O	000124-25-4	44
4			Tridecanoic acid	214	C13H26O2	000638-53-9	42
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040521\
Data File : BP005178.D
Acq On : 05 Apr 2021 14:49
Operator : CG/JU
Sample : M1897-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

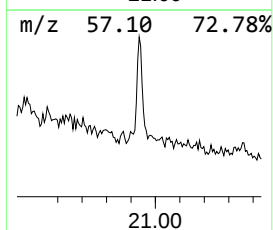
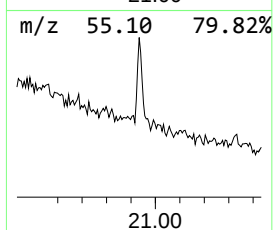
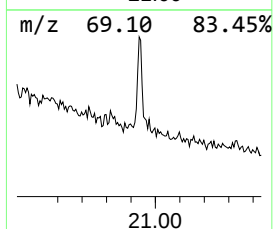
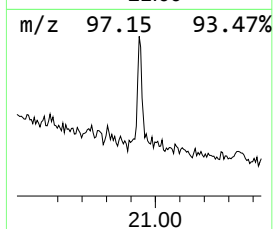
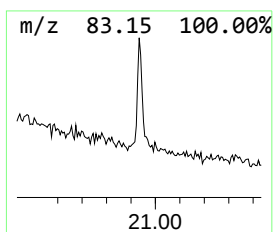
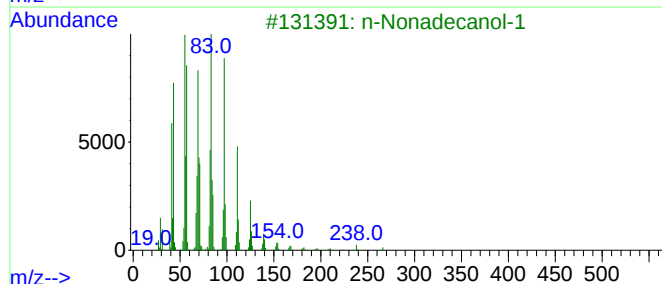
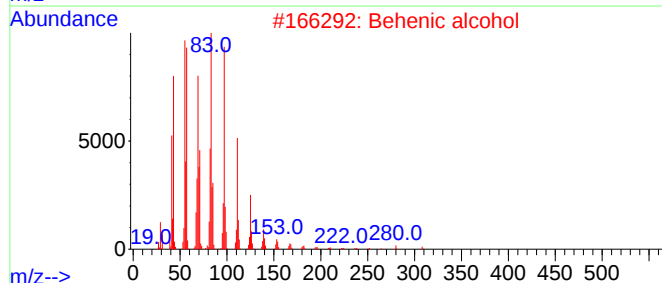
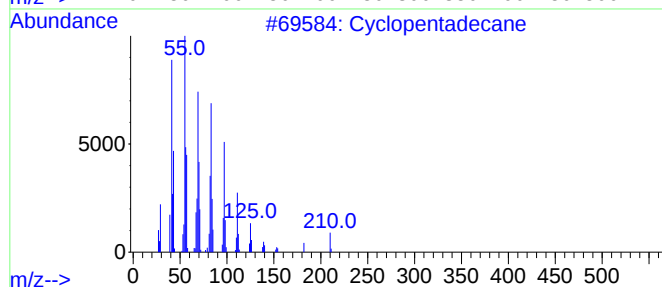
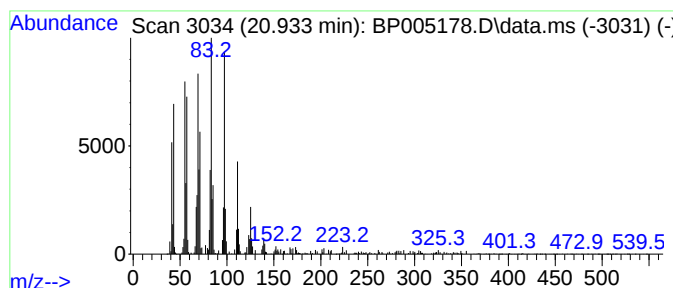
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	12.09 ng	211845	Chrysene-d12	21.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040521\
Data File : BP005178.D
Acq On : 05 Apr 2021 14:49
Operator : CG/JU
Sample : M1897-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.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-...	13.128	2.7	ng	43734	3	14.357	327100	20.0
Decahydro-4,4,8...	13.893	4.5	ng	74413	3	14.357	327100	20.0
unknown14.00	14.004	2.2	ng	36557	3	14.357	327100	20.0
unknown14.09	14.098	11.3	ng	185176	3	14.357	327100	20.0
1-(2-Hydroxyeth...	14.187	16.6	ng	270883	3	14.357	327100	20.0
Tetracosane	14.887	8.4	ng	138235	3	14.357	327100	20.0
unknown15.15	15.151	18.0	ng	294829	3	14.357	327100	20.0
n-Hexadecanoic ...	18.028	13.6	ng	319778	4	17.128	471181	20.0
Cyclopentadecane	20.933	12.1	ng	211845	5	21.221	350339	20.0