

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040521\
 Data File : BP005182.D
 Acq On : 05 Apr 2021 17:05
 Operator : CG/JU
 Sample : M1894-02
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 0156-AMENDED-CP-COMP

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: BP005182.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.840	293	298	307	rVB	245597	321825	28.10%	5.053%
2	5.299	370	376	383	rBV	235140	333977	29.16%	5.243%
3	6.881	637	645	657	rBV	370154	567426	49.54%	8.908%
4	7.005	660	666	674	rVB	34327	56129	4.90%	0.881%
5	7.699	777	784	792	rBV	97653	150354	13.13%	2.360%
6	8.857	974	981	990	rBV	225961	371195	32.41%	5.828%
7	9.093	1016	1021	1027	rVB	8100	12951	1.13%	0.203%
8	9.216	1035	1042	1047	rBV	19928	34608	3.02%	0.543%
9	10.493	1251	1259	1266	rBV	112488	195026	17.03%	3.062%
10	12.969	1672	1680	1691	rBV	526468	772157	67.42%	12.123%
11	13.816	1819	1824	1834	rBV	21708	31168	2.72%	0.489%
12	14.257	1895	1899	1904	rVB3	8618	14139	1.23%	0.222%
13	14.357	1910	1916	1924	rVB	169980	246517	21.52%	3.870%
14	15.857	2163	2171	2179	rBV	194044	288362	25.18%	4.527%
15	16.086	2205	2210	2215	rBV2	18317	29575	2.58%	0.464%
16	16.881	2340	2345	2352	rBV3	23926	39651	3.46%	0.623%
17	17.116	2378	2385	2390	rBV	205629	298670	26.08%	4.689%
18	17.157	2390	2392	2398	rVB	15352	20769	1.81%	0.326%
19	17.245	2403	2407	2415	rVB2	19198	31653	2.76%	0.497%
20	18.016	2534	2538	2547	rBV2	51498	67793	5.92%	1.064%
21	19.139	2725	2729	2736	rVB	60574	76832	6.71%	1.206%
22	19.257	2746	2749	2752	rBV3	13986	16214	1.42%	0.255%
23	19.492	2785	2789	2798	rVB	49969	76589	6.69%	1.202%
24	19.692	2818	2823	2829	rBV	1003260	1145340	100.00%	17.981%
25	19.975	2868	2871	2877	rVB3	22325	31755	2.77%	0.499%
26	20.074	2885	2888	2892	rVB2	18469	21193	1.85%	0.333%
27	20.933	3030	3034	3041	rVB4	80130	110700	9.67%	1.738%
28	21.216	3076	3082	3086	rBV2	348306	464557	40.56%	7.293%
29	21.251	3086	3088	3092	rVB	43606	48327	4.22%	0.759%
30	22.804	3348	3352	3357	rBV2	45355	81975	7.16%	1.287%
31	23.504	3465	3471	3477	rVB	230546	412184	35.99%	6.471%

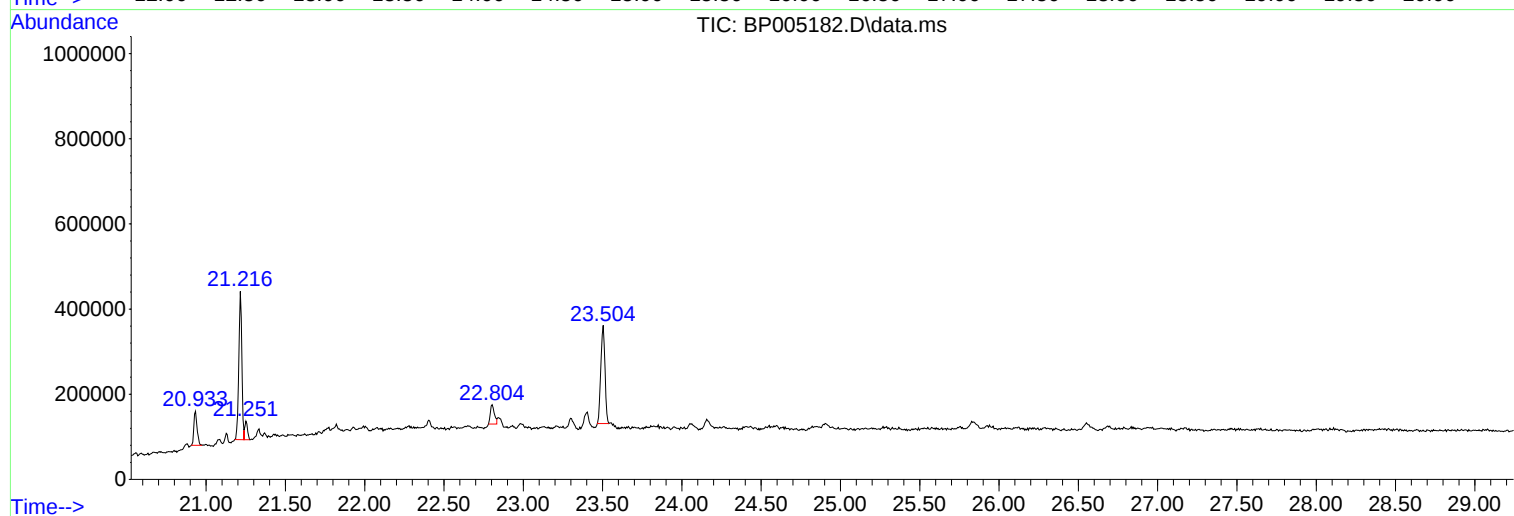
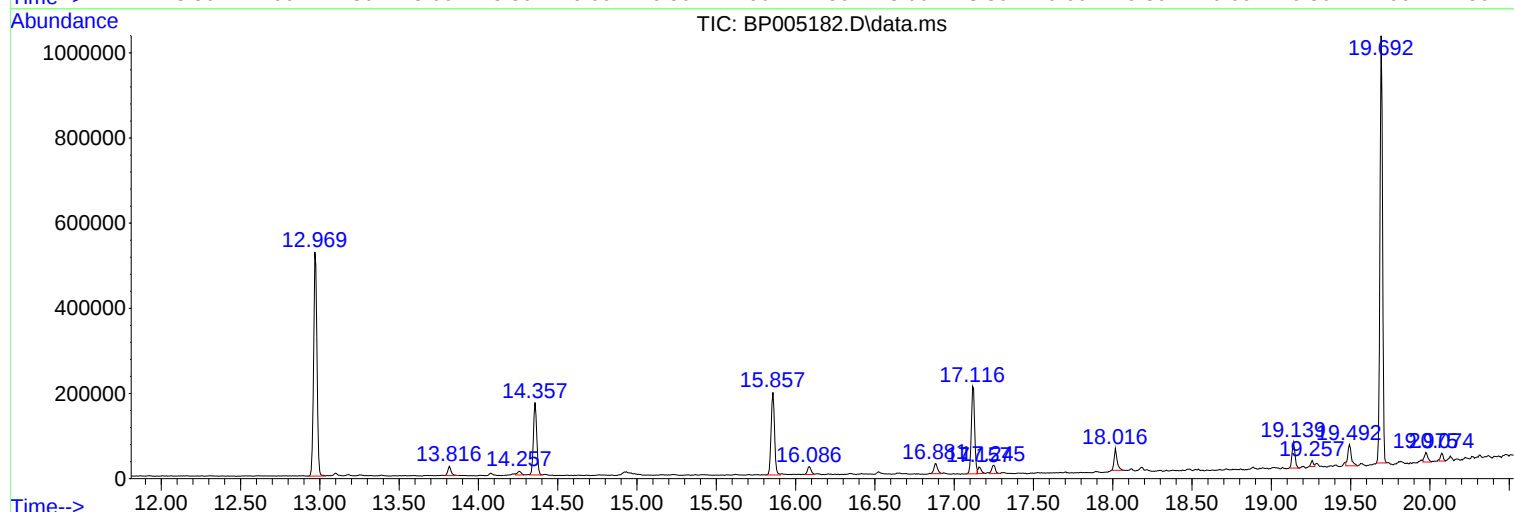
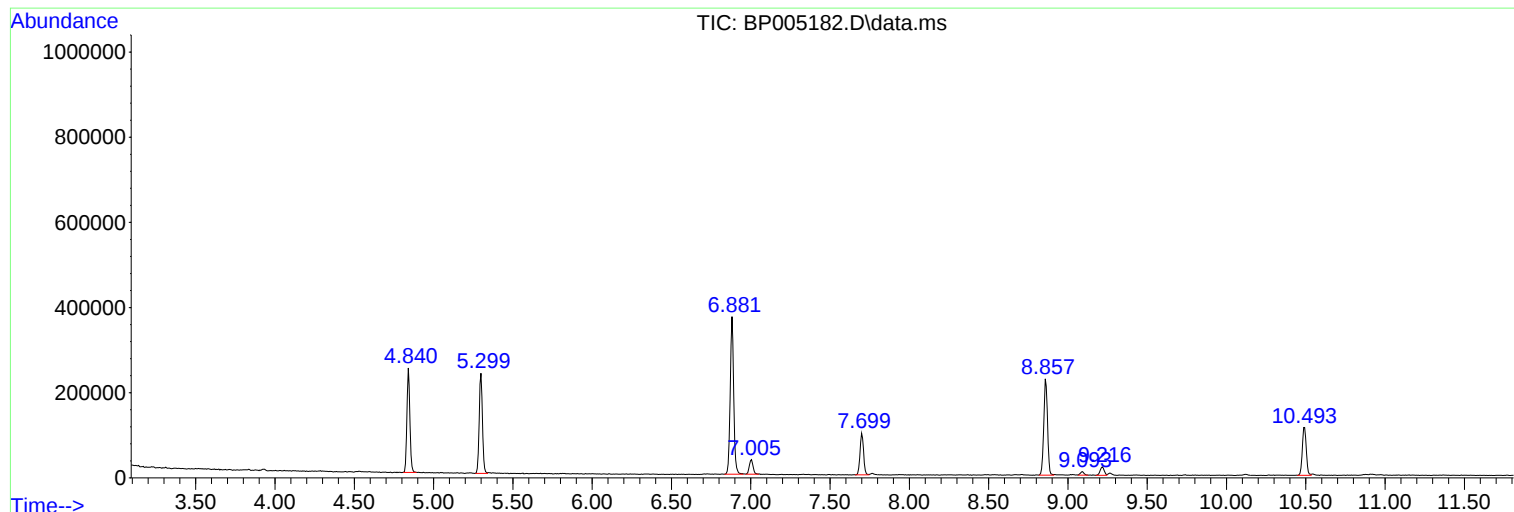
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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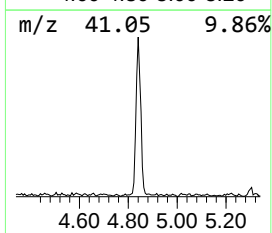
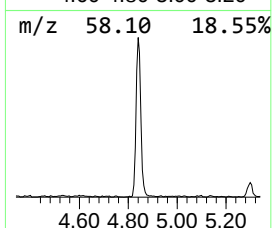
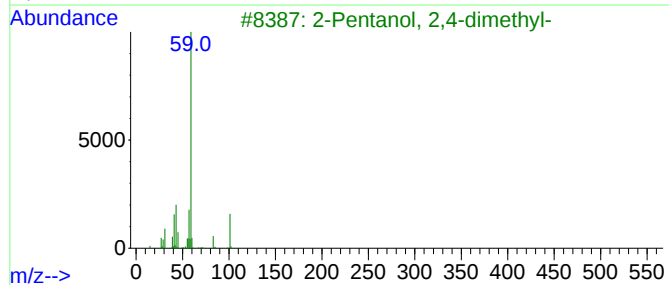
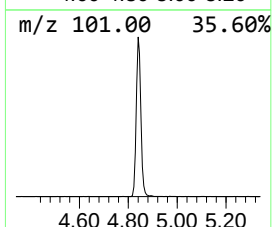
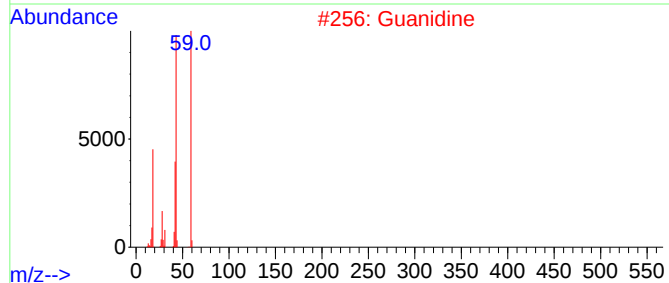
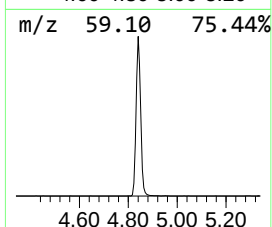
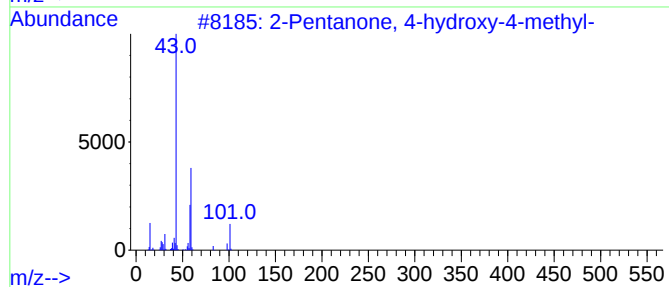
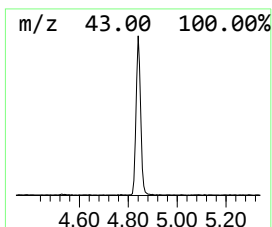
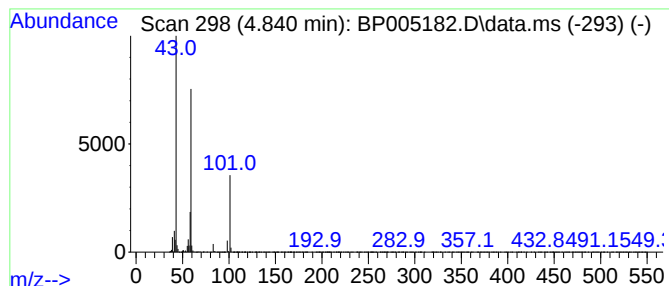
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.840	42.81 ng	321825	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Guanidine	59	CH5N3	000113-00-8	50		
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	39		
4	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	28		
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	28		



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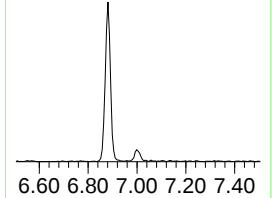
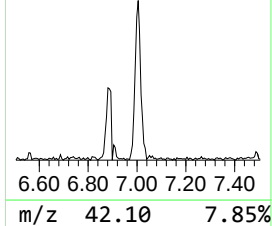
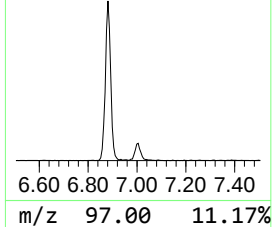
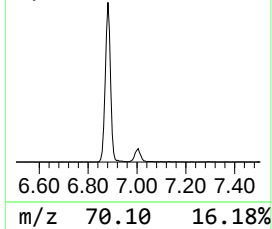
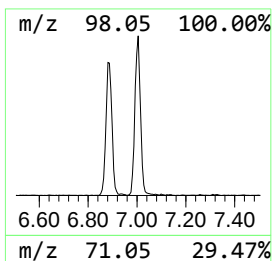
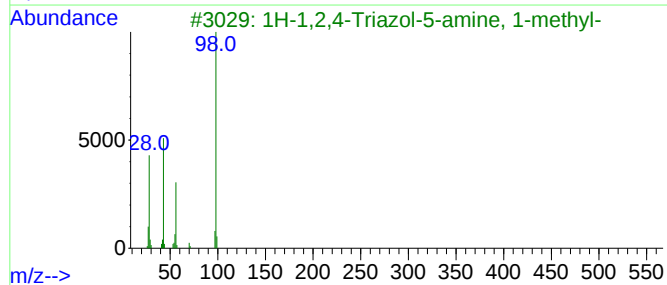
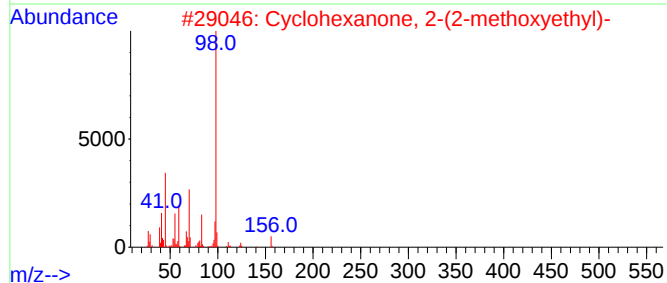
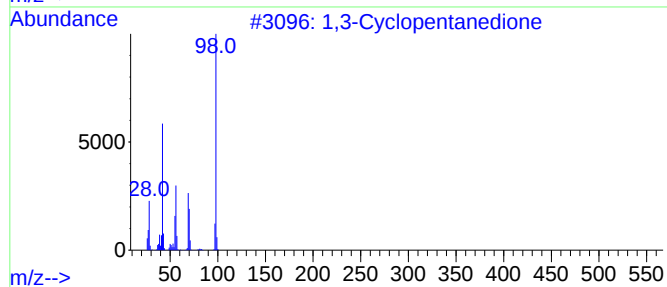
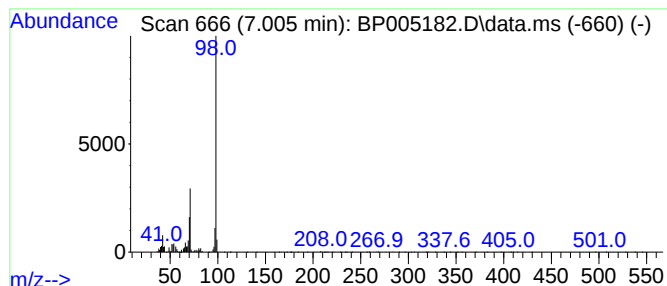
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Cyclopentanedione Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.005	7.47 ng	56129	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclopentanedione	98	C5H6O2	003859-41-4	64
2			Cyclohexanone, 2-(2-methoxyethyl)-	156	C9H16O2	129786-15-8	64
3			1H-1,2,4-Triazol-5-amine, 1-methyl-	98	C3H6N4	015795-39-8	53
4			Pyrido[2,3-d]pyrimidine-2,4(1H,3...	385	C16H21Cl2N5O2	1000265-65-2	53
5			Sulpiride	341	C15H23N3O4S	015676-16-1	50



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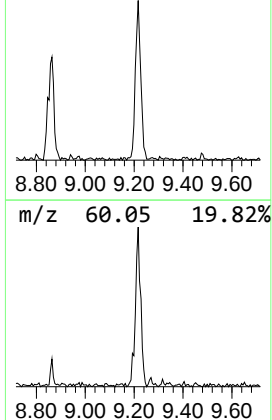
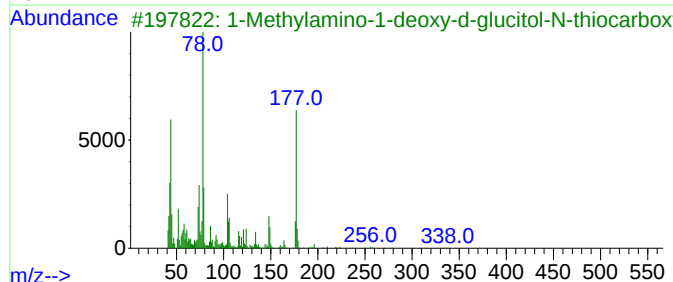
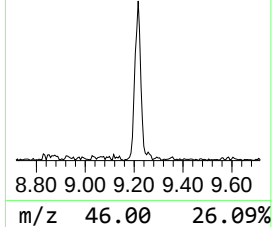
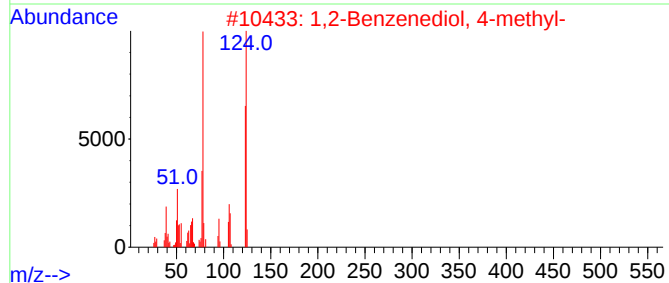
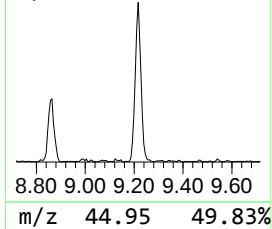
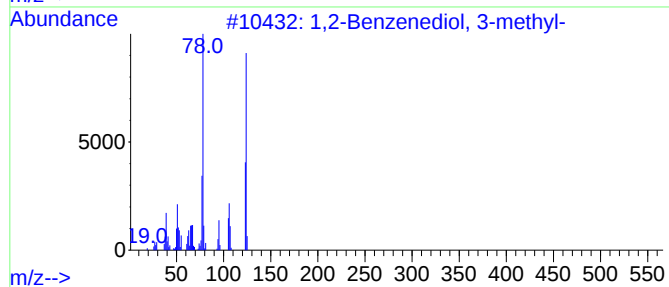
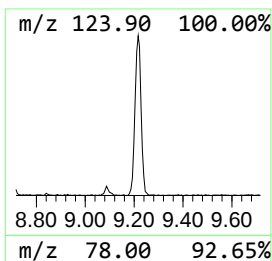
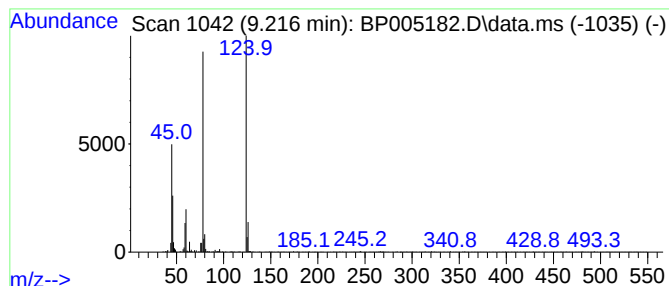
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown9.21 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	3.55 ng	34608	Naphthalene-d8	10.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenediol, 3-methyl-	124	C7H8O2	000488-17-5	45
2			1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	45
3			1-Methylamino-1-deoxy-d-glucitol...	372	C15H24N4O5S	071605-30-6	33
4			Benzene	78	C6H6	000071-43-2	9
5			2H-Pyrido[1,2-a][1,3,5]triazine...	349	C17H14F3N3O2	1000276-51-2	9



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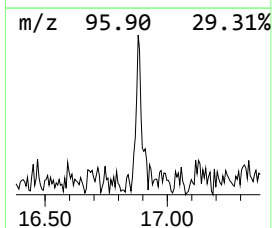
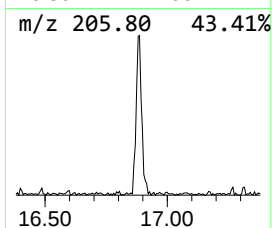
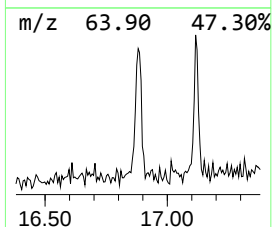
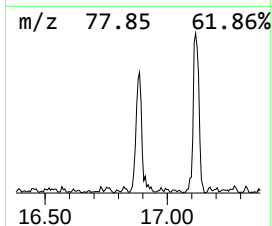
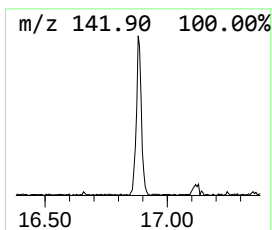
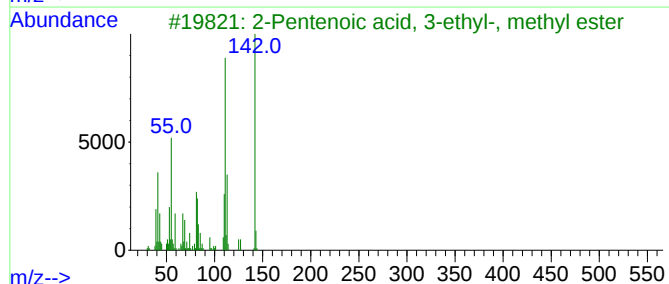
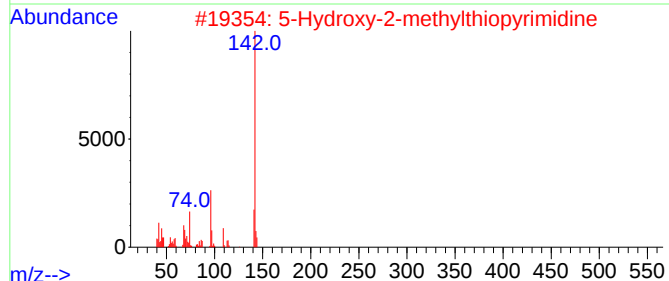
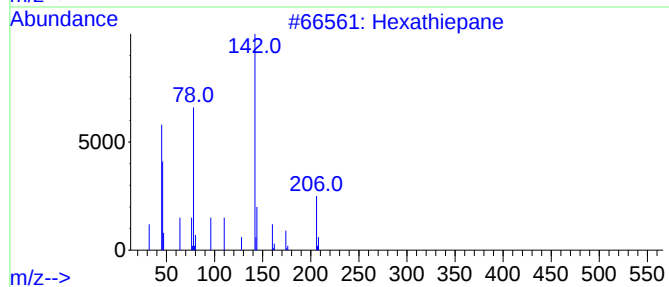
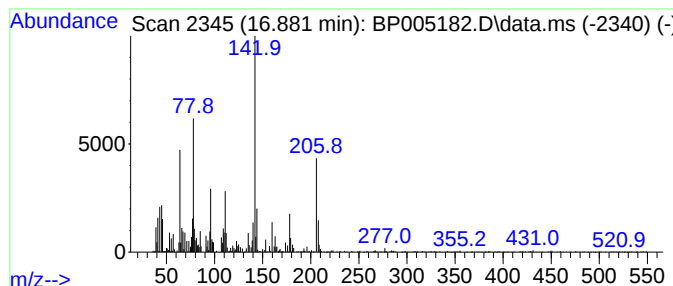
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Peak Number 4 unknown16.88 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.881	2.66 ng	39651	Phenanthrene-d10	17.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexathiepane	206	CH2S6	017233-71-5	43
2			5-Hydroxy-2-methylthiopyrimidine	142	C5H6N2OS	004874-33-3	11
3			2-Pentenoic acid, 3-ethyl-, meth...	142	C8H14O2	013979-17-4	10
4			3-Amino-3-(2,4-difluoro-phenyl)-...	201	C9H9F2NO2	1000297-15-7	10
5			1-[2-Dibutylamino-1-hydroxyethyl]...	417	C24H29Cl2NO	030737-76-9	10



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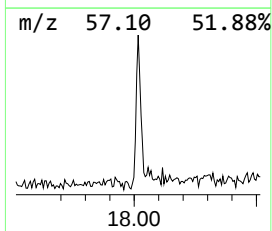
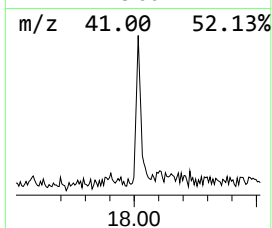
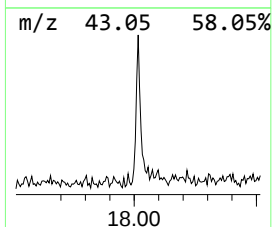
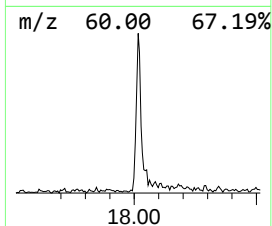
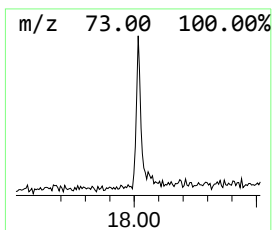
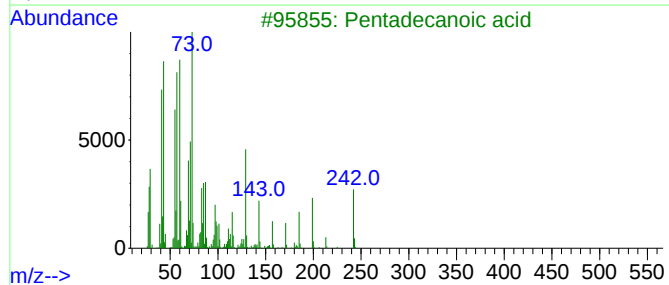
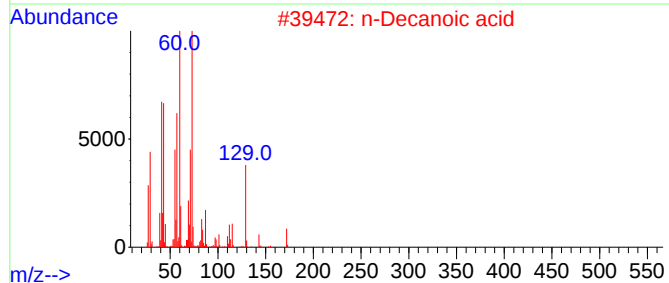
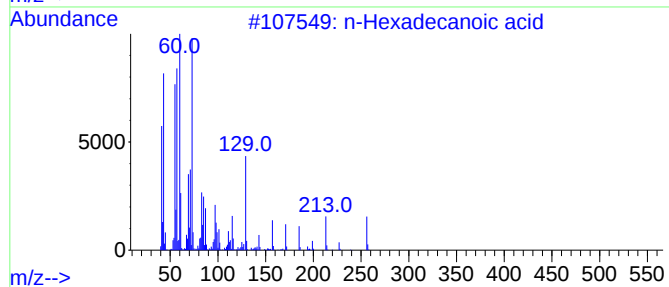
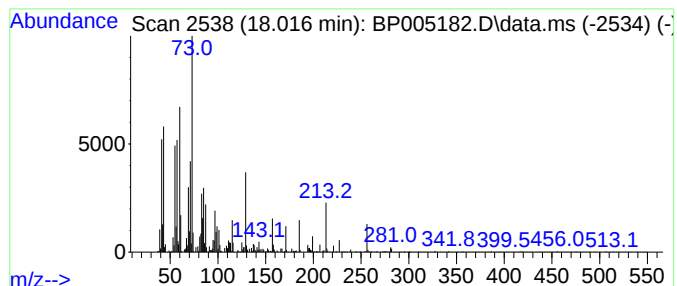
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.016	4.54 ng	67793	Phenanthrene-d10	17.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			n-Decanoic acid	172	C10H20O2	000334-48-5	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4			Tridecanoic acid	214	C13H26O2	000638-53-9	58
5			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	35



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0156-AMENDED-CP-COMP

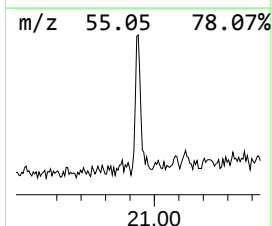
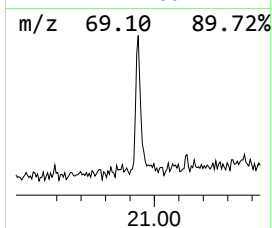
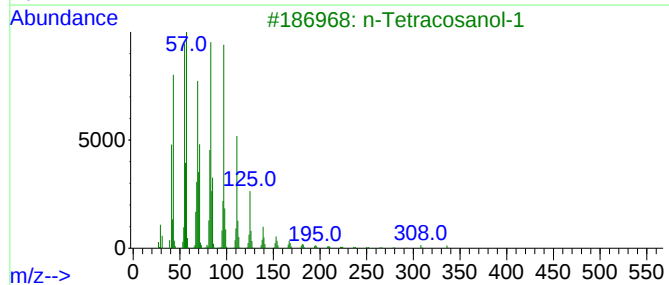
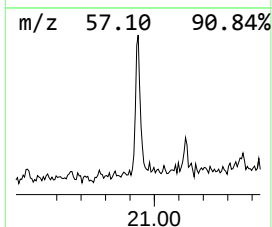
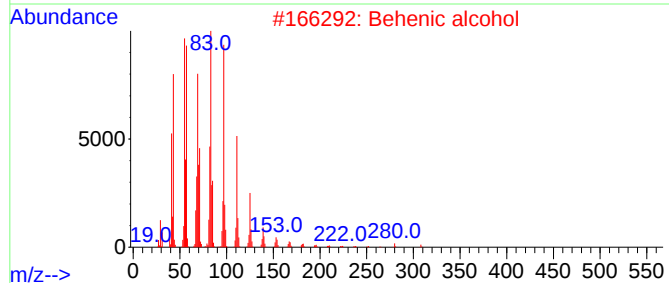
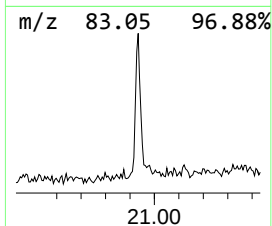
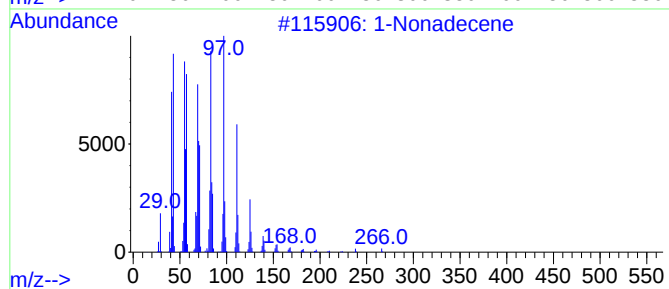
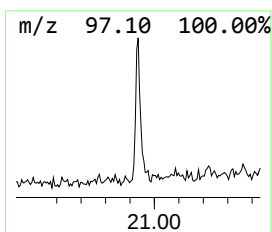
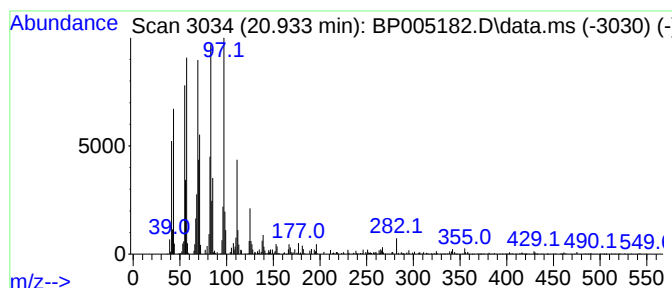
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	4.77 ng	110700	Chrysene-d12	21.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	95
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			1-Heptacosanol	396	C27H56O	002004-39-9	92
5			1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040521\
Data File : BP005182.D
Acq On : 05 Apr 2021 17:05
Operator : CG/JU
Sample : M1894-02
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
0156-AMENDED-CP-COMP

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-...	4.840	42.8	ng	321825	1	7.699	150354	20.0
1,3-Cyclopentan...	7.005	7.5	ng	56129	1	7.699	150354	20.0
unknown9.21	9.216	3.5	ng	34608	2	10.487	195026	20.0
unknown16.88	16.881	2.7	ng	39651	4	17.116	298670	20.0
n-Hexadecanoic ...	18.016	4.5	ng	67793	4	17.116	298670	20.0
1-Nonadecene	20.933	4.8	ng	110700	5	21.216	464557	20.0