

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
 Data File : BP005160.D
 Acq On : 02 Apr 2021 15:37
 Operator : CG/JU
 Sample : M1836-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 B2-0-2

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: BP005160.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.693	97	103	112	rVB2	17344	30147	2.12%	0.352%
2	3.787	113	119	125	rBV2	22696	39086	2.75%	0.456%
3	4.846	295	299	308	rVB	45392	67815	4.78%	0.791%
4	5.234	360	365	370	rVB	35314	50068	3.53%	0.584%
5	5.305	370	377	383	rVV	538996	778901	54.86%	9.084%
6	5.381	383	390	399	rVB2	33098	70865	4.99%	0.826%
7	5.728	442	449	455	rVB6	8643	16294	1.15%	0.190%
8	6.193	523	528	536	rVB5	8056	16001	1.13%	0.187%
9	6.687	603	612	619	rBV2	24323	49367	3.48%	0.576%
10	6.881	635	645	658	rBV	516483	876496	61.74%	10.223%
11	7.352	716	725	731	rBV	71840	112553	7.93%	1.313%
12	7.705	777	785	792	rBV	122878	199706	14.07%	2.329%
13	7.816	799	804	810	rVB	20200	34234	2.41%	0.399%
14	7.940	819	825	831	rBV4	11456	25052	1.76%	0.292%
15	8.069	840	847	853	rBV	10374	15860	1.12%	0.185%
16	8.340	888	893	906	rVB6	12264	29574	2.08%	0.345%
17	8.722	951	958	963	rBV4	7343	17519	1.23%	0.204%
18	8.805	967	972	975	rBV	12373	18001	1.27%	0.210%
19	8.863	975	982	990	rVB	312539	512986	36.13%	5.983%
20	10.493	1248	1259	1265	rBV	159863	275540	19.41%	3.214%
21	12.975	1671	1681	1690	rBV	761065	1088563	76.67%	12.696%
22	13.769	1812	1816	1820	rBV4	13173	19440	1.37%	0.227%
23	13.816	1820	1824	1827	rBV	25816	36148	2.55%	0.422%
24	14.181	1883	1886	1895	rVB7	8457	17743	1.25%	0.207%
25	14.357	1906	1916	1923	rBV	243849	349290	24.60%	4.074%
26	15.857	2164	2171	2178	rBV	535189	762226	53.69%	8.890%
27	17.116	2379	2385	2391	rBV	255758	384429	27.08%	4.484%
28	18.022	2534	2539	2548	rBV	102132	151058	10.64%	1.762%
29	19.139	2726	2729	2733	rVB	28345	32077	2.26%	0.374%
30	19.257	2745	2749	2754	rBV2	38179	52993	3.73%	0.618%
31	19.692	2818	2823	2829	rBV	1185739	1419770	100.00%	16.559%
32	20.933	3030	3034	3042	rVB2	159618	219651	15.47%	2.562%
33	20.998	3043	3045	3049	rVB	34168	37532	2.64%	0.438%
34	21.216	3078	3082	3087	rBV	324797	384419	27.08%	4.483%
35	23.498	3465	3470	3478	rVB2	202878	382758	26.96%	4.464%

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

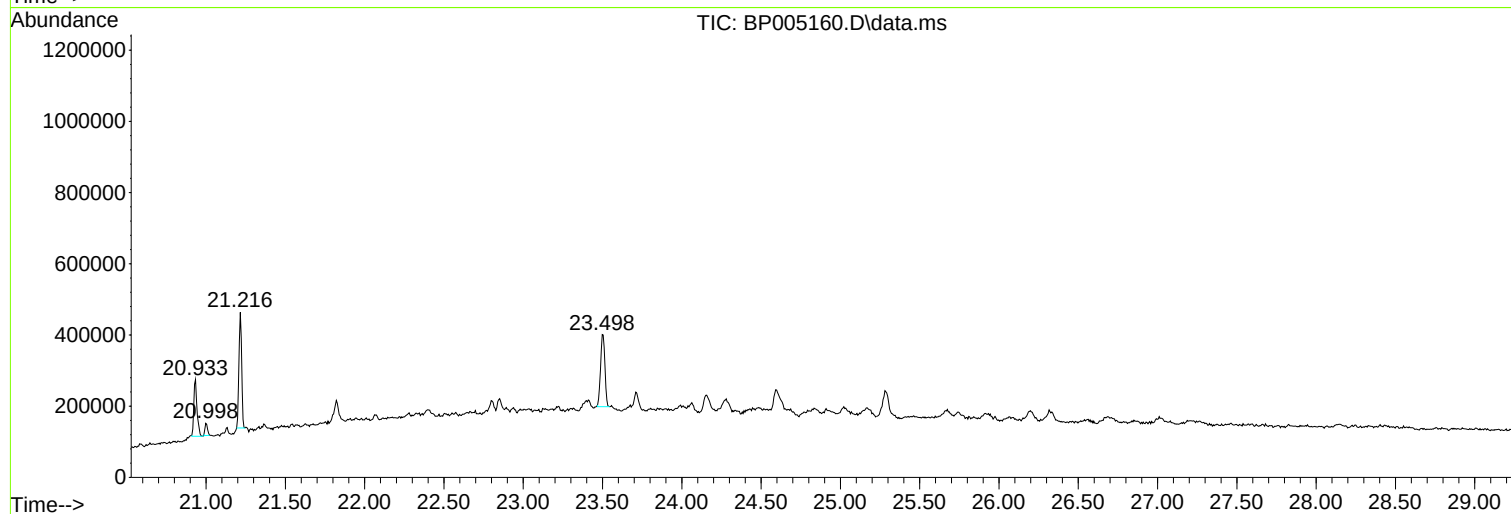
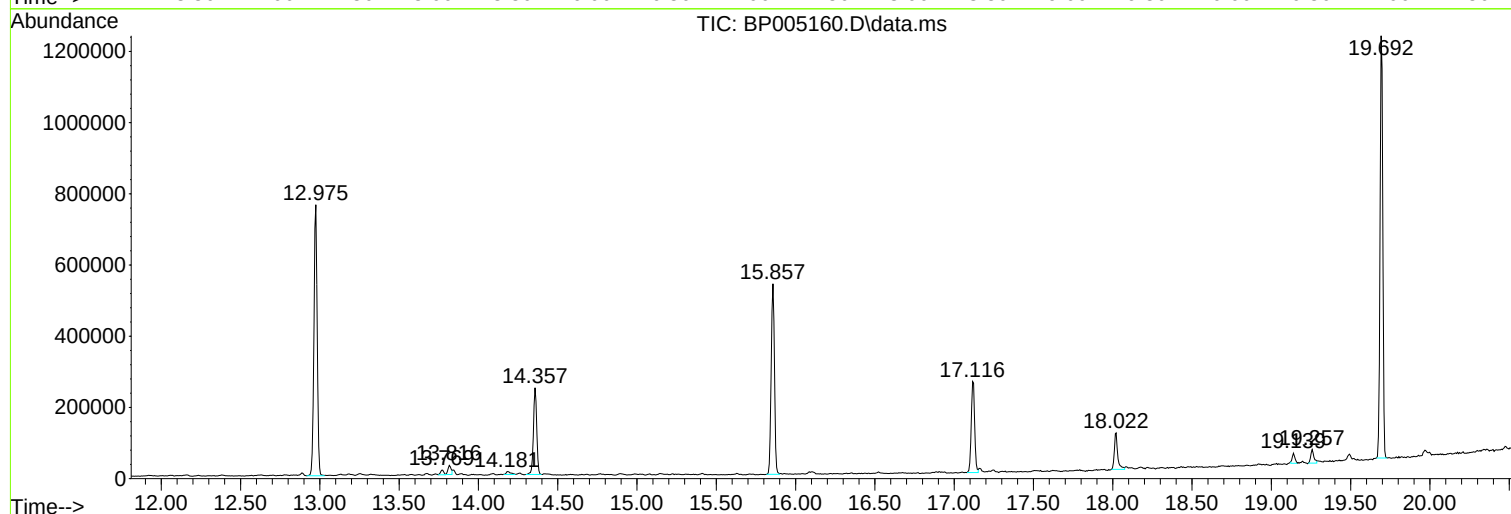
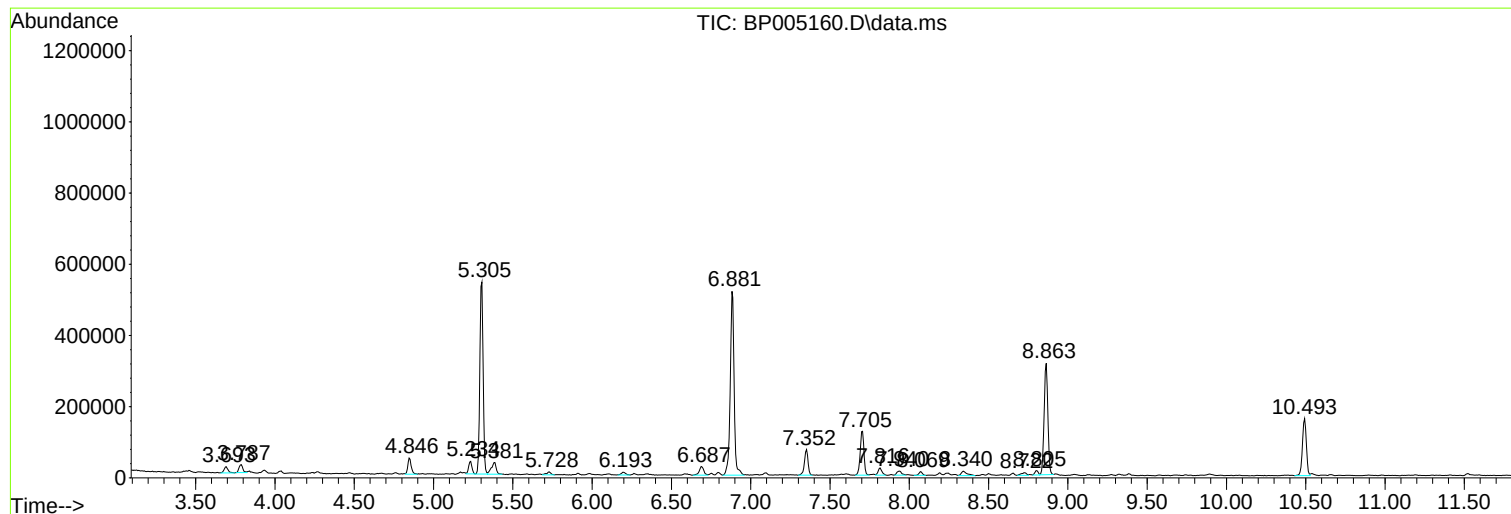
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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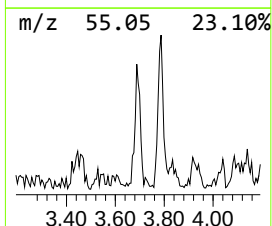
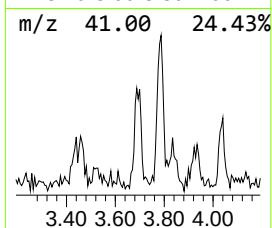
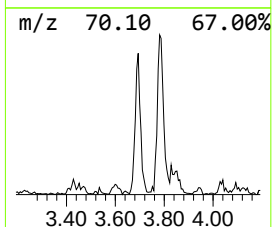
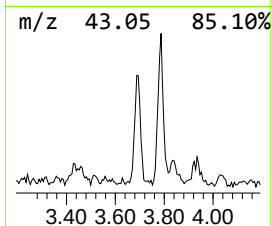
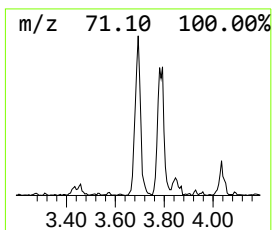
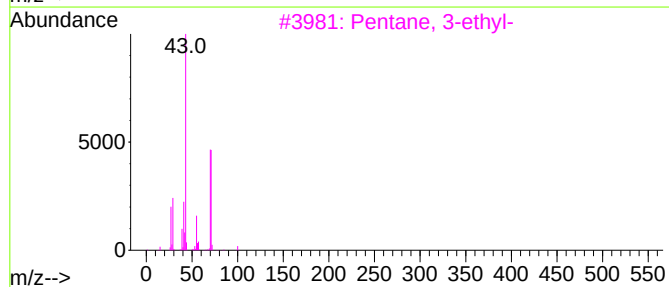
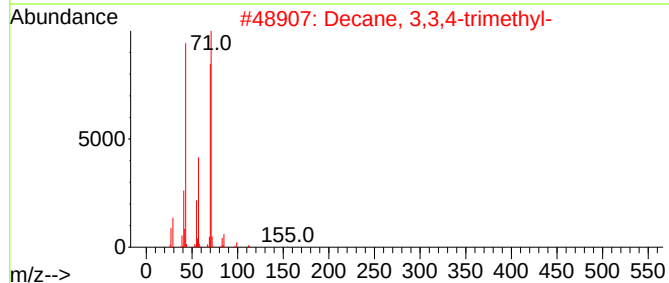
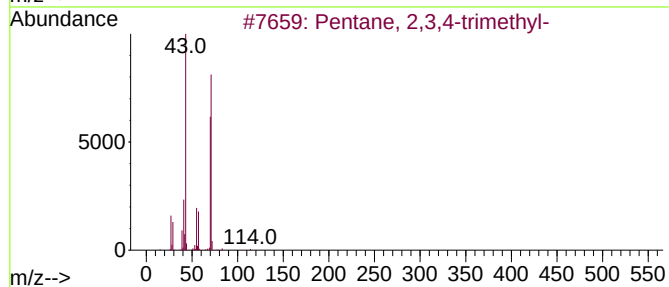
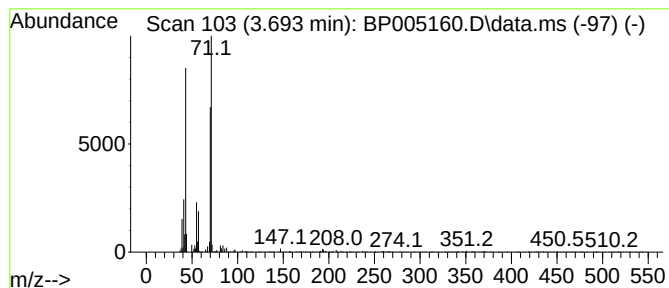
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Pentane, 2,3,4-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.693	3.02 ng	30147	1,4-Dichlorobenzene-d4	7.699

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
2		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	56
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	50
4		Decane, 3,3,6-trimethyl-	184	C13H28	062338-14-1	50
5		Heptane, 4-methyl-	114	C8H18	000589-53-7	50



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ClientSampleId :
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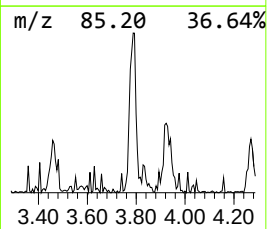
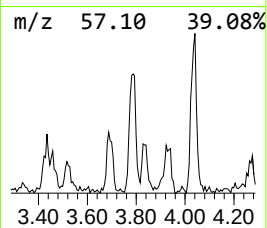
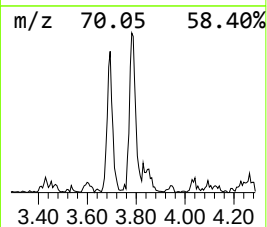
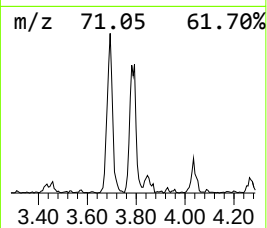
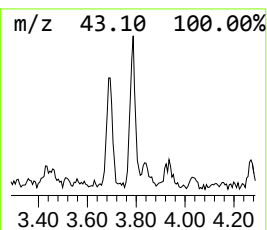
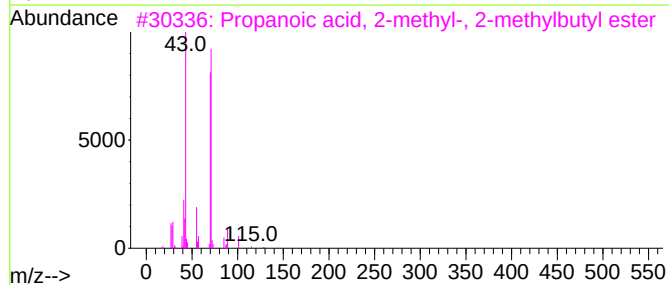
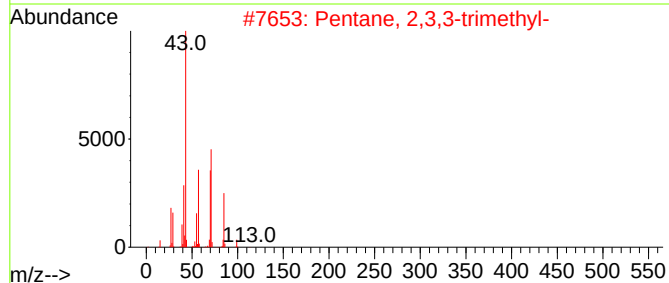
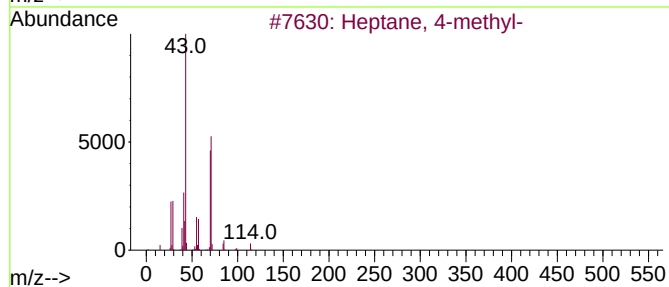
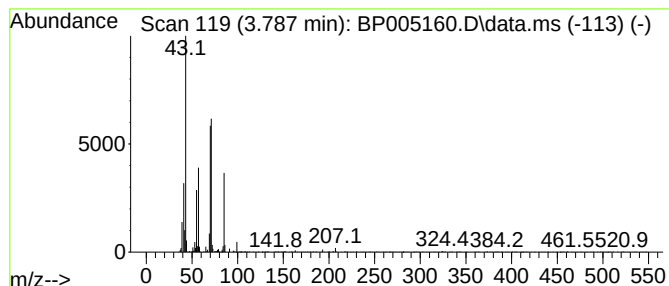
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Heptane, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.787	3.91 ng	39086	1,4-Dichlorobenzene-d4	7.699

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
2		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	59
3		Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	59
4		3,3-Dimethyl-2-pentanol	116	C7H16O	019781-24-9	59
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59



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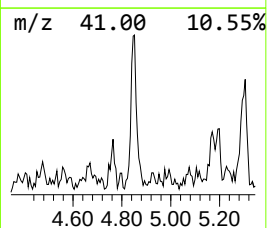
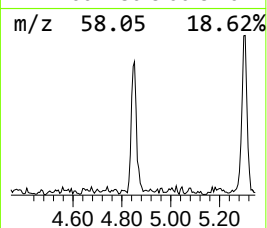
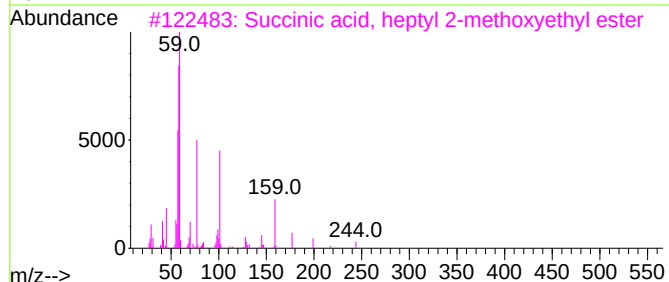
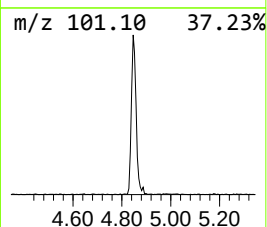
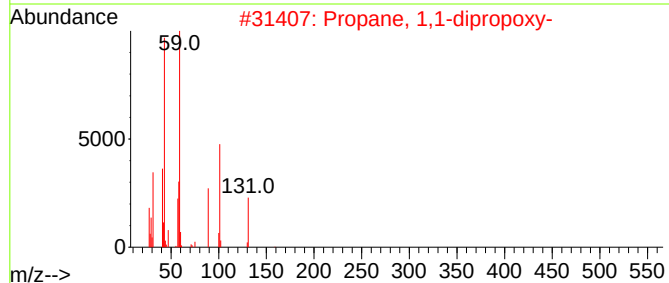
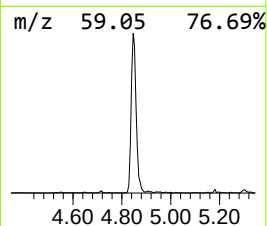
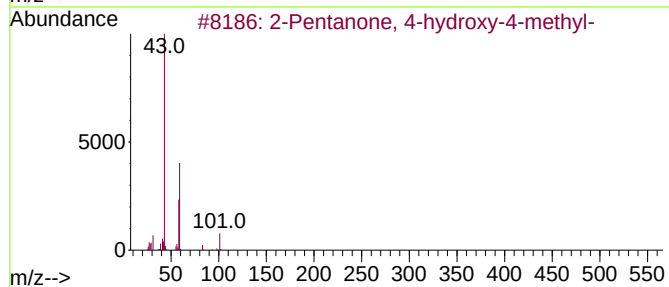
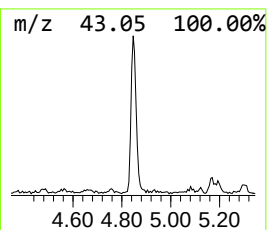
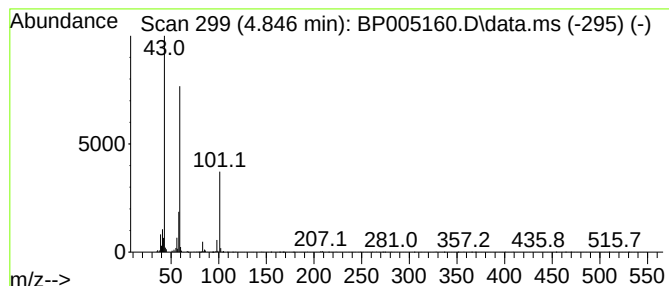
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.846	6.79 ng	67815	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	64		
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	39		
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	36		
4	2,3-Dimethyloxirane-2-carboxylic...	130	C6H10O3	1000306-64-4	36		
5	Tetraglyme	222	C10H22O5	000143-24-8	33		



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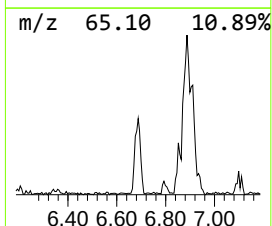
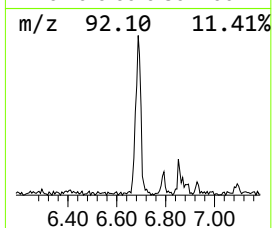
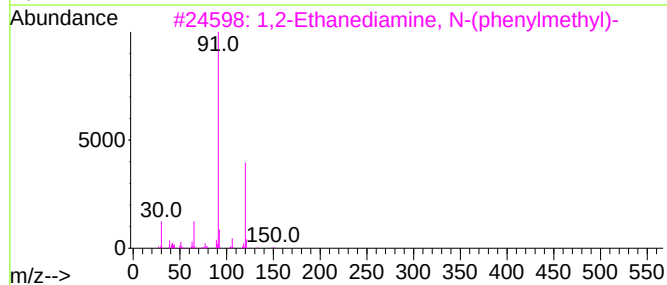
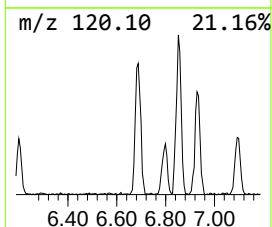
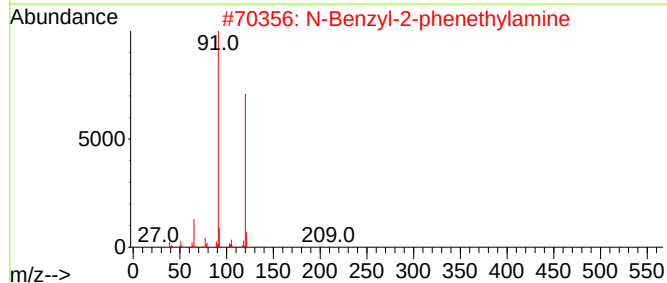
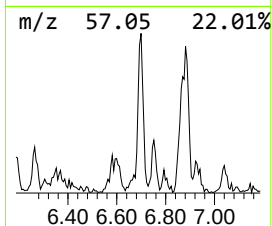
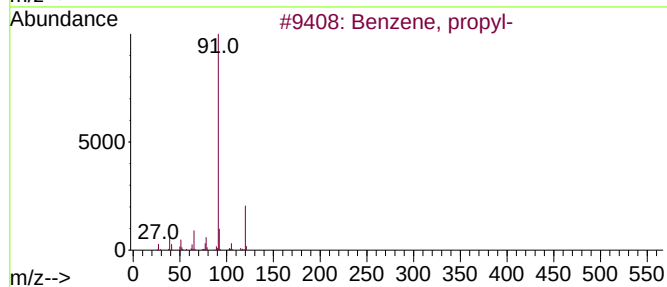
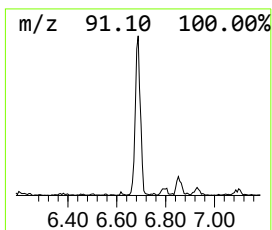
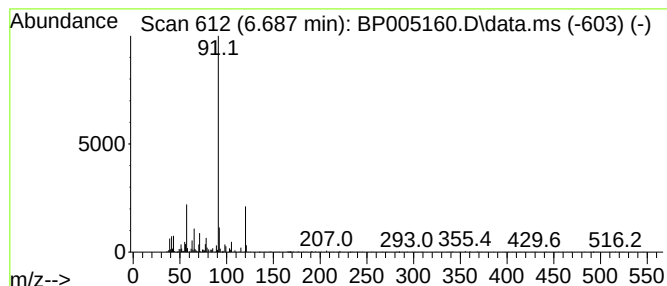
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.687	4.94 ng	49367	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	87
2			N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	64
3			1,2-Ethanediamine, N-(phenylmeth...	150	C9H14N2	004152-09-4	59
4			Propanenitrile, 3-[(phenylmethyl...	160	C10H12N2	000706-03-6	59
5			1,2-Ethanediamine, N,N'-bis(phen...	240	C16H20N2	000140-28-3	59



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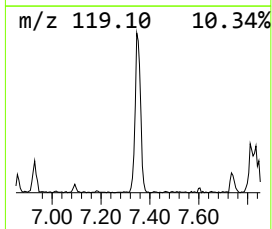
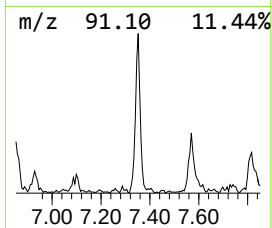
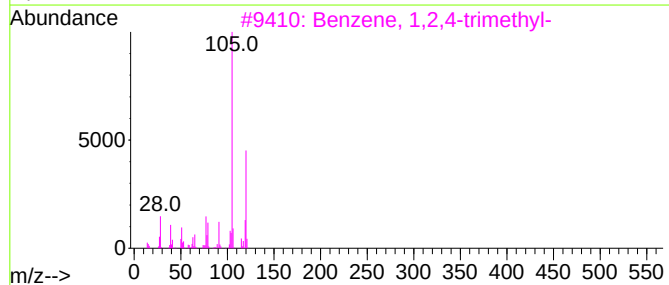
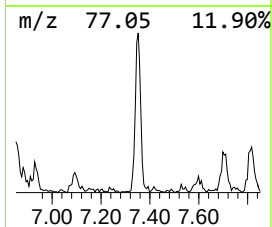
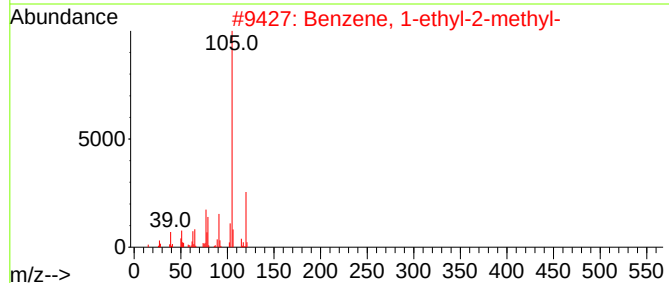
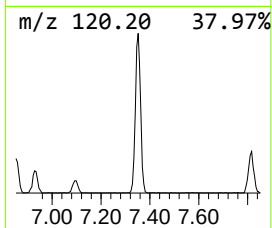
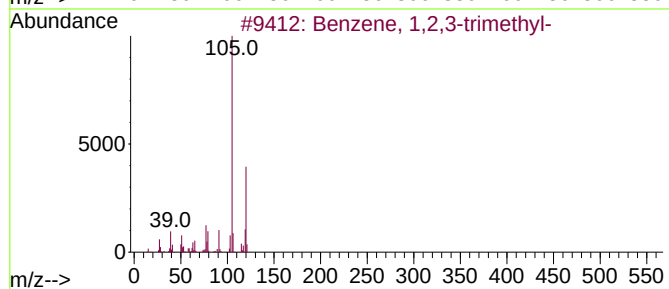
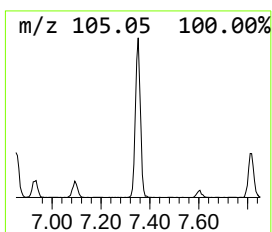
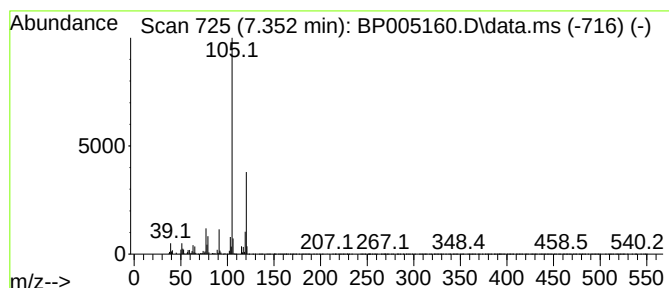
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.352	11.27 ng	112553	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	93
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005160.D
Acq On : 02 Apr 2021 15:37
Operator : CG/JU
Sample : M1836-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

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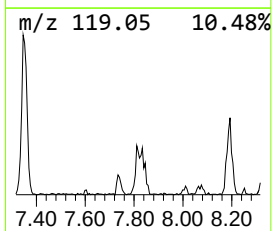
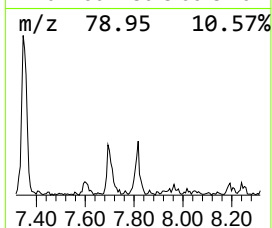
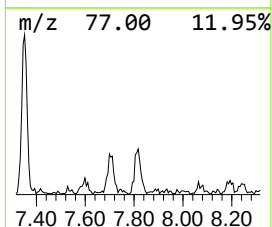
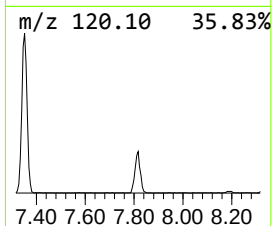
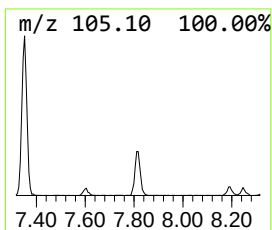
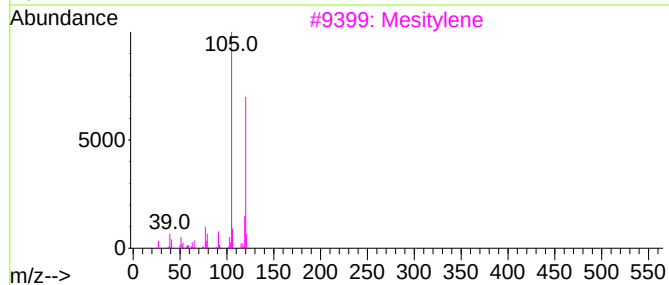
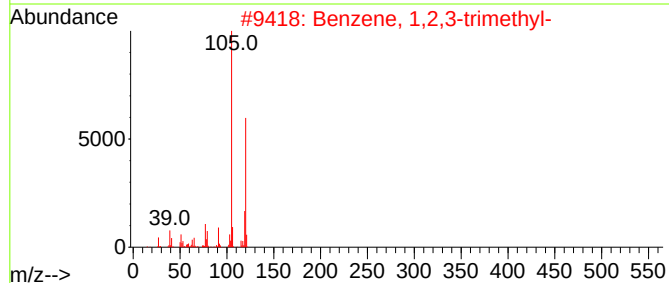
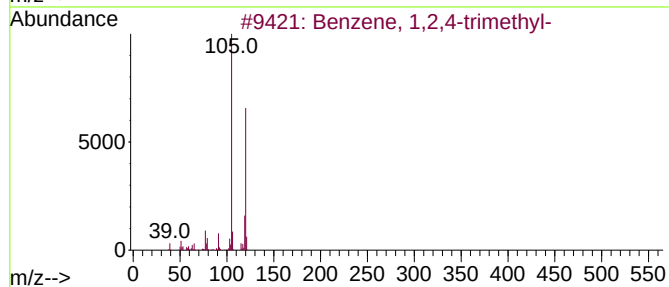
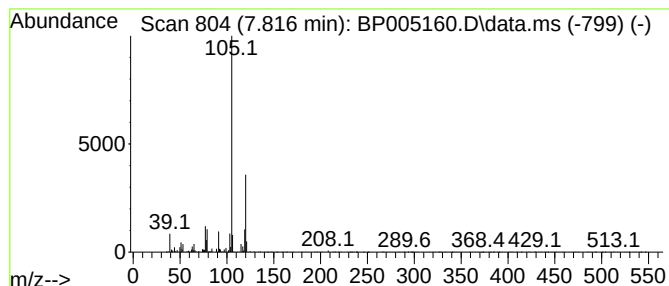
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzene, 1,2,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.816	3.43 ng	34234	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005160.D
Acq On : 02 Apr 2021 15:37
Operator : CG/JU
Sample : M1836-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
B2-0-2

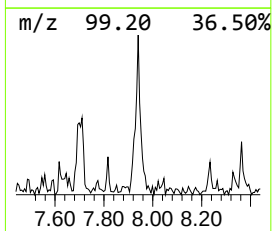
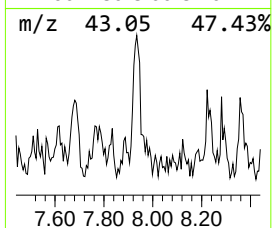
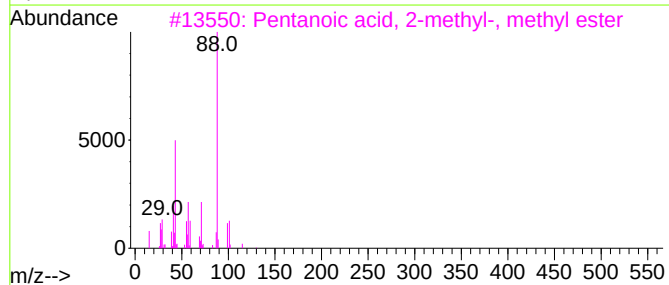
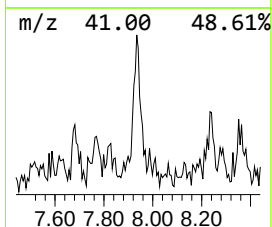
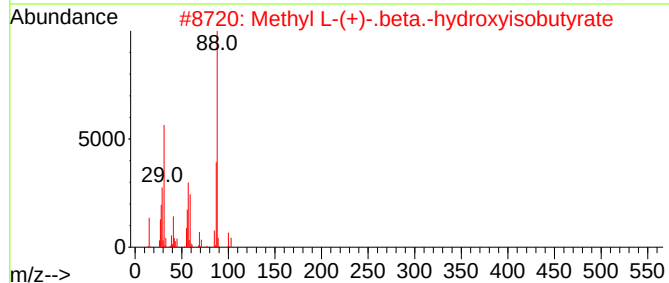
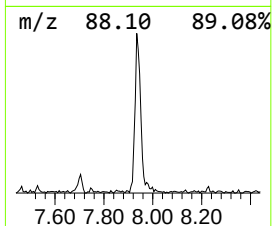
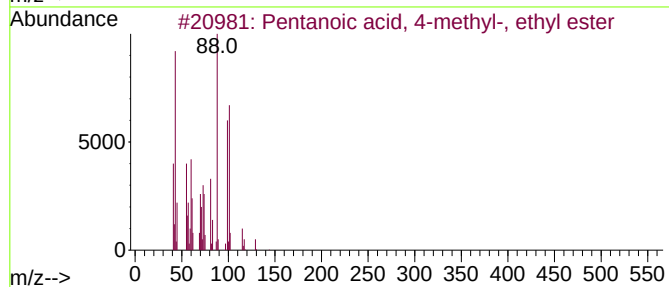
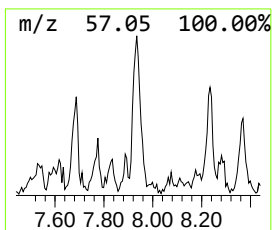
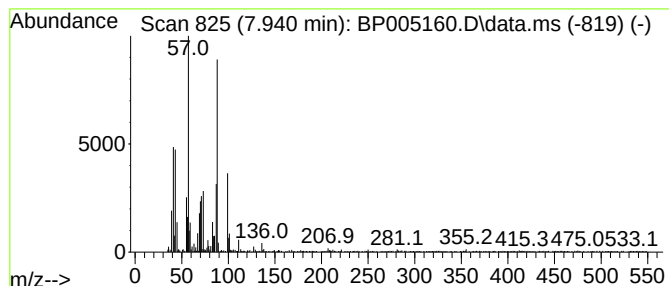
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentanoic acid, 4-methyl-, ... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.940	2.51 ng	25052	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanoic acid, 4-methyl-, ethyl...	144	C8H16O2	025415-67-2	59
2			Methyl L-(+)-.beta.-hydroxyisobu...	118	C5H10O3	080657-57-4	50
3			Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	47
4			9-Decenoic acid, 2,4-dimethyl-, ...	212	C13H24O2	031183-23-0	46
5			9-Decenoic acid, 2,4-dimethyl-, ...	212	C13H24O2	031183-24-1	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005160.D
Acq On : 02 Apr 2021 15:37
Operator : CG/JU
Sample : M1836-03
Misc :
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Instrument :
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ClientSampleId :
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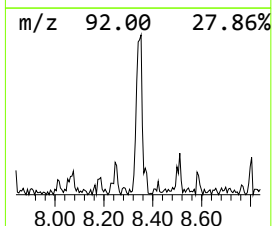
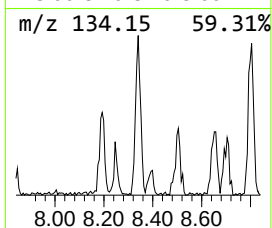
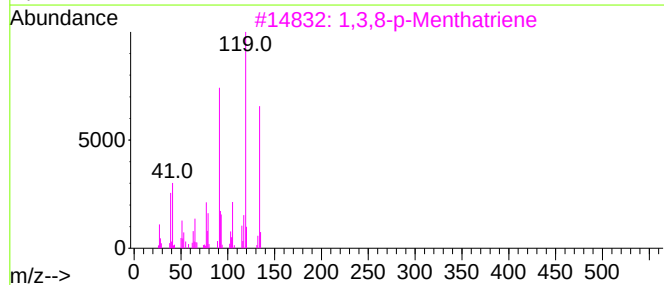
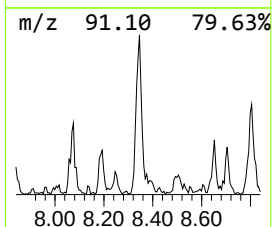
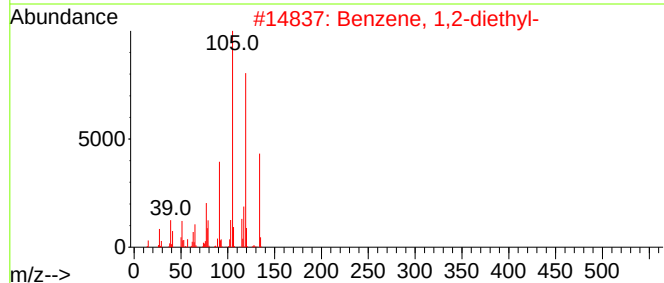
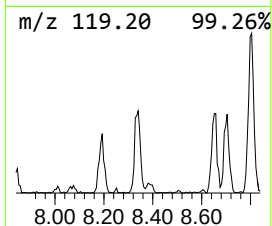
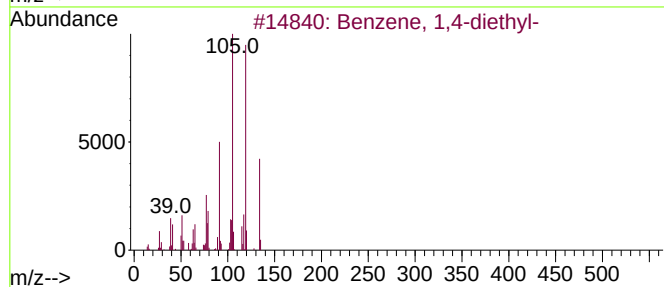
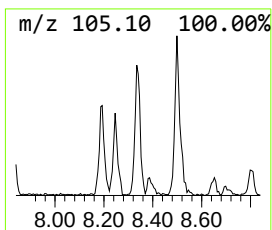
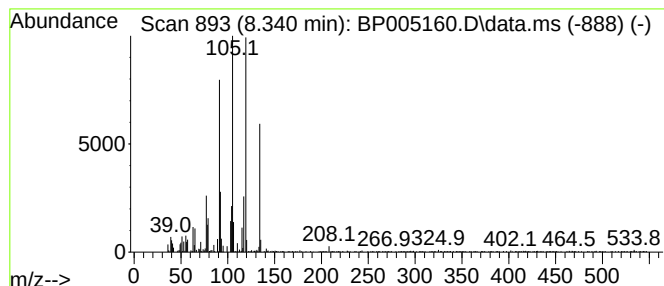
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzene, 1,4-diethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.340	2.96 ng	29574	1,4-Dichlorobenzene-d4	7.699

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	76
2			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	70
3			1,3,8-p-Menthatriene	134	C10H14	018368-95-1	64
4			Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	58
5			5H-5-Methyl-6,7-dihydrocyclopent...	134	C8H10N2	023747-48-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005160.D
Acq On : 02 Apr 2021 15:37
Operator : CG/JU
Sample : M1836-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

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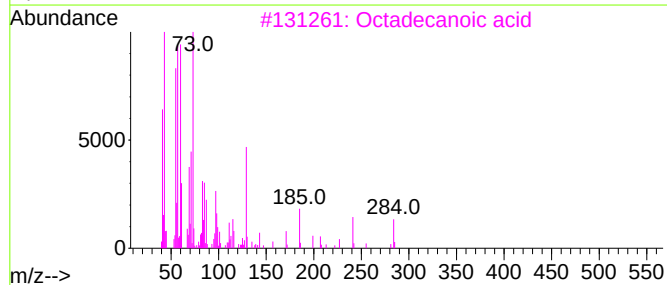
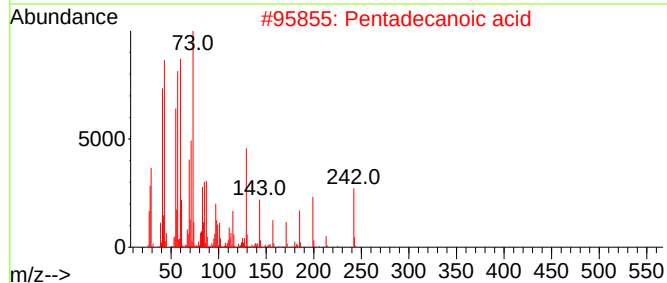
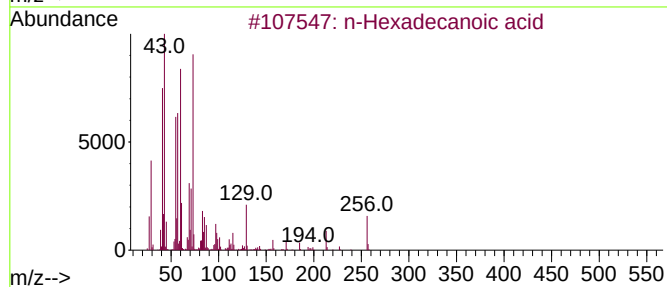
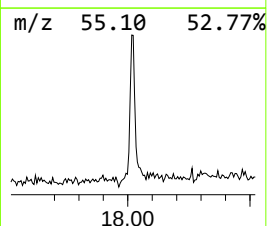
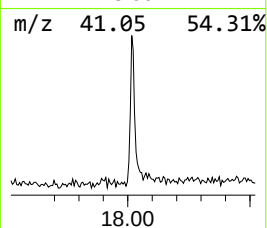
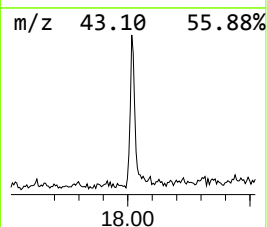
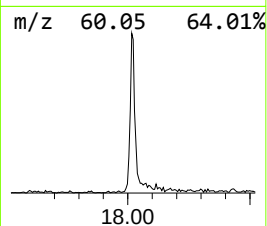
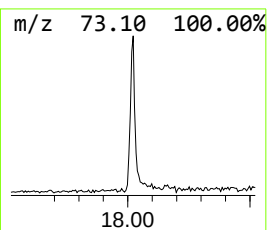
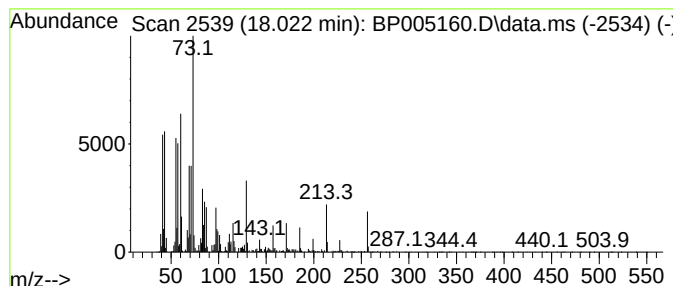
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	7.86 ng	151058	Phenanthrene-d10	17.122

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Octadecanoic acid	284	C18H36O2	000057-11-4	58
4			Tridecanoic acid	214	C13H26O2	000638-53-9	49
5			Estra-1,3,5(10)-trien-17.β-ol	256	C18H24O	002529-64-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
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Sample : M1836-03
Misc :
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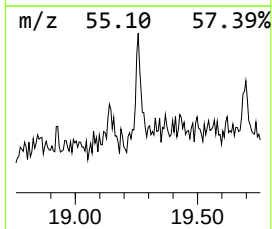
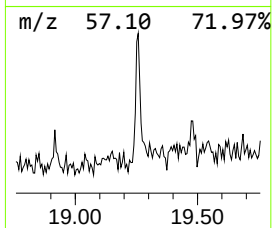
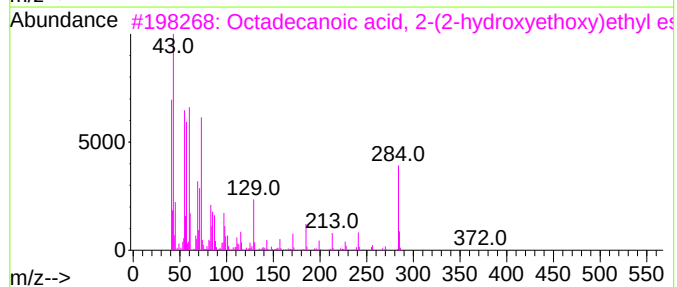
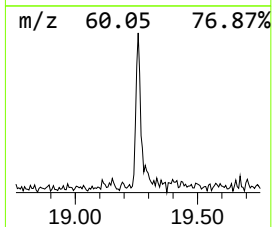
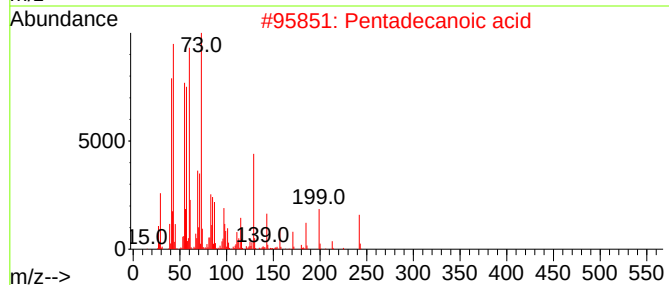
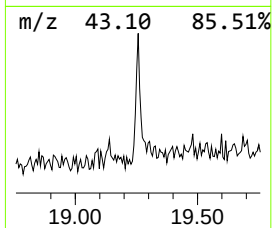
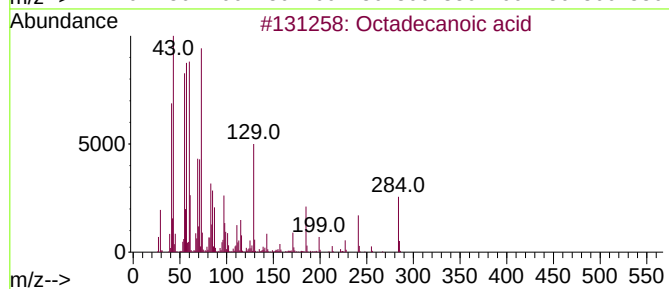
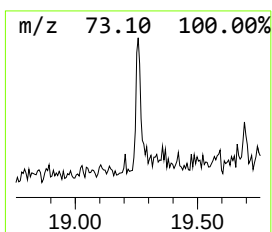
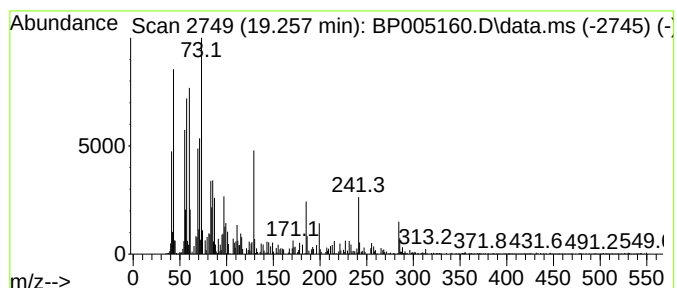
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.257	2.76 ng	52993	Chrysene-d12	21.216	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	46
5	Undecanoic acid	186	C11H22O2	000112-37-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005160.D
Acq On : 02 Apr 2021 15:37
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ALS Vial : 13 Sample Multiplier: 1

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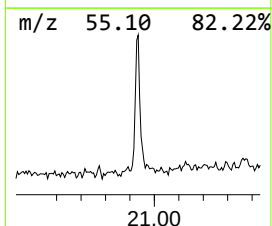
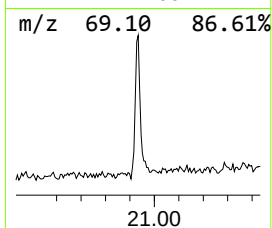
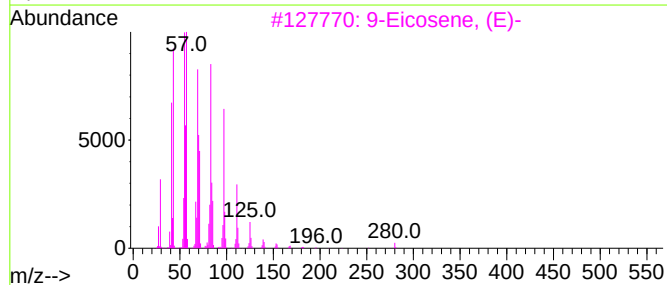
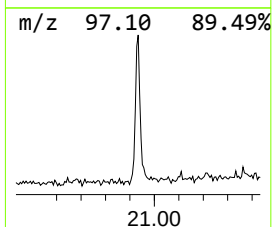
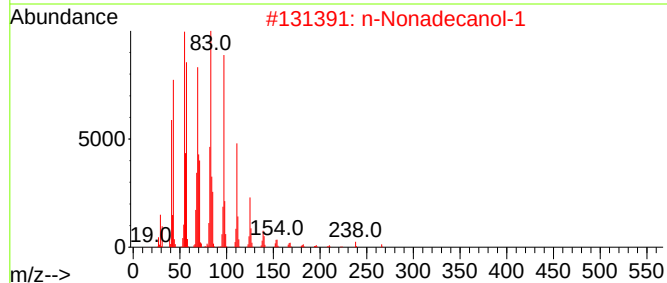
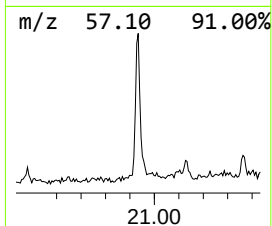
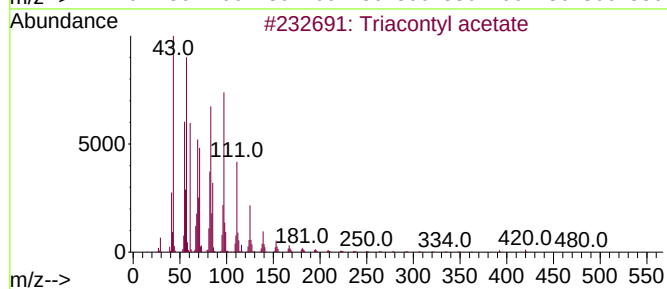
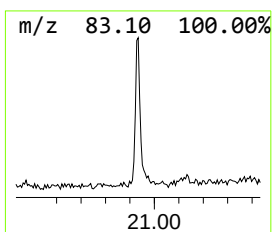
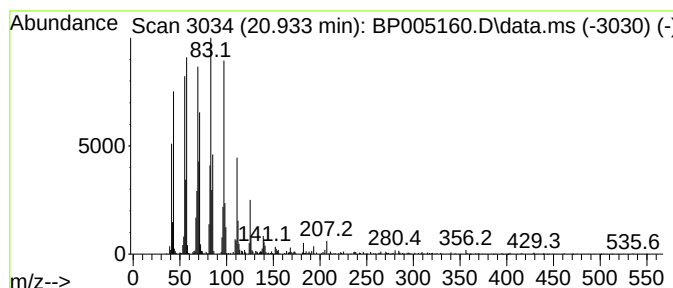
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Triacontyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.933	11.43 ng	219651	Chrysene-d12	21.216

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontyl acetate	480	C32H64O2	041755-58-2	94
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4		E-14-Hexadecenal	238	C16H30O	330207-53-9	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040221\
Data File : BP005160.D
Acq On : 02 Apr 2021 15:37
Operator : CG/JU
Sample : M1836-03
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\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
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Heptane, 4-methyl-	3.787	3.9	ng	39086	1	7.699	199706	20.0
2-Pentanone, 4-...	4.846	6.8	ng	67815	1	7.699	199706	20.0
Benzene, propyl-	6.687	4.9	ng	49367	1	7.699	199706	20.0
Benzene, 1,2,3-...	7.352	11.3	ng	112553	1	7.699	199706	20.0
Benzene, 1,2,4-...	7.816	3.4	ng	34234	1	7.699	199706	20.0
Pentanoic acid,...	7.940	2.5	ng	25052	1	7.699	199706	20.0
Benzene, 1,4-di...	8.340	3.0	ng	29574	1	7.699	199706	20.0
n-Hexadecanoic ...	18.022	7.9	ng	151058	4	17.122	384429	20.0
Octadecanoic acid	19.257	2.8	ng	52993	5	21.216	384419	20.0
Triacetyl acetate	20.933	11.4	ng	219651	5	21.216	384419	20.0