

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060421\
 Data File : BP005710.D
 Acq On : 04 Jun 2021 13:37
 Operator : CG/JU
 Sample : M2611-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 T-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.540	411	417	427	rBV	2065592	2973888	36.85%	7.110%
2	7.146	682	690	705	rBV	1987687	3184111	39.45%	7.613%
3	7.981	824	832	840	rBV	444003	695343	8.62%	1.662%
4	9.146	1020	1030	1042	rBV	1208021	2062285	25.55%	4.931%
5	10.199	1201	1209	1217	rVB	164939	272502	3.38%	0.652%
6	10.563	1264	1271	1284	rBV	295247	547813	6.79%	1.310%
7	10.787	1301	1309	1315	rBV	562222	931703	11.54%	2.228%
8	12.246	1548	1557	1570	rBV	3430223	5314332	65.85%	12.706%
9	13.234	1716	1725	1740	rBV	3215110	4685821	58.06%	11.203%
10	13.457	1757	1763	1768	rBV	174824	244674	3.03%	0.585%
11	14.604	1948	1958	1965	rBV	831201	1227311	15.21%	2.934%
12	16.092	2204	2211	2230	rBV	2997478	4509119	55.87%	10.781%
13	17.345	2418	2424	2430	rBV	1072494	1531205	18.97%	3.661%
14	18.228	2569	2574	2582	rBV	201957	295291	3.66%	0.706%
15	19.345	2760	2764	2770	rBV	67732	97223	1.20%	0.232%
16	19.698	2821	2824	2833	rVB2	62805	94239	1.17%	0.225%
17	19.892	2851	2857	2862	rBV	6669018	8070748	100.00%	19.296%
18	20.516	2959	2963	2967	rBV	305100	376025	4.66%	0.899%
19	21.122	3062	3066	3073	rBV2	375365	559174	6.93%	1.337%
20	21.416	3111	3116	3121	rBV	1505792	2025884	25.10%	4.844%
21	23.857	3525	3531	3539	rVB2	1051857	2126905	26.35%	5.085%

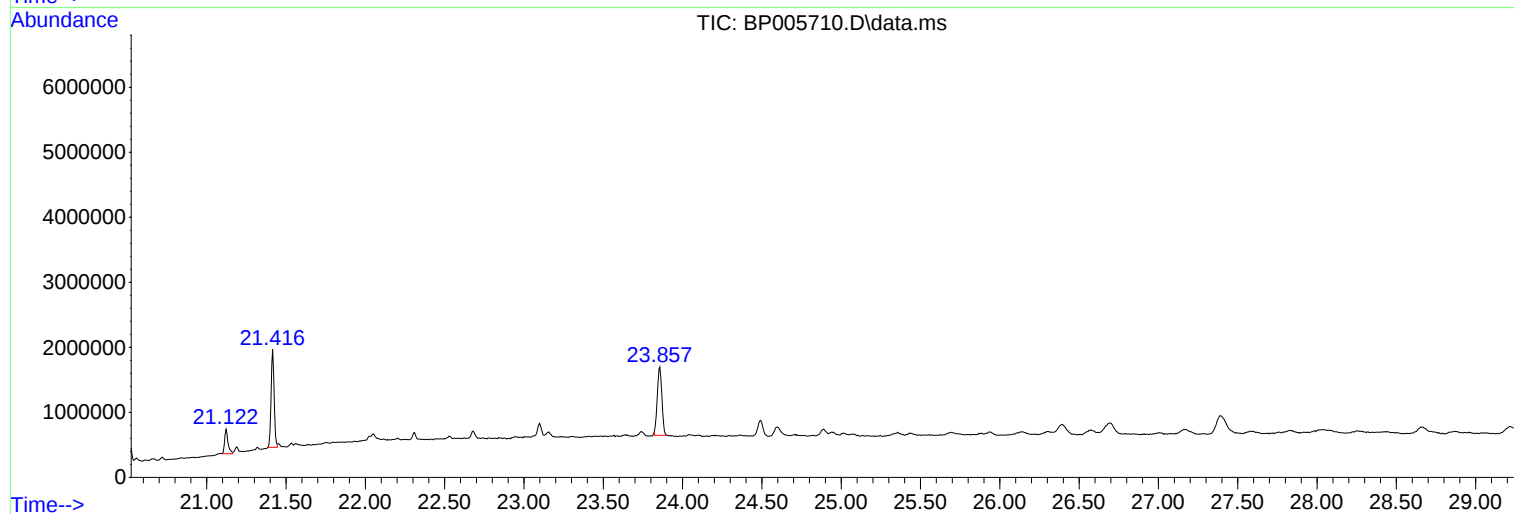
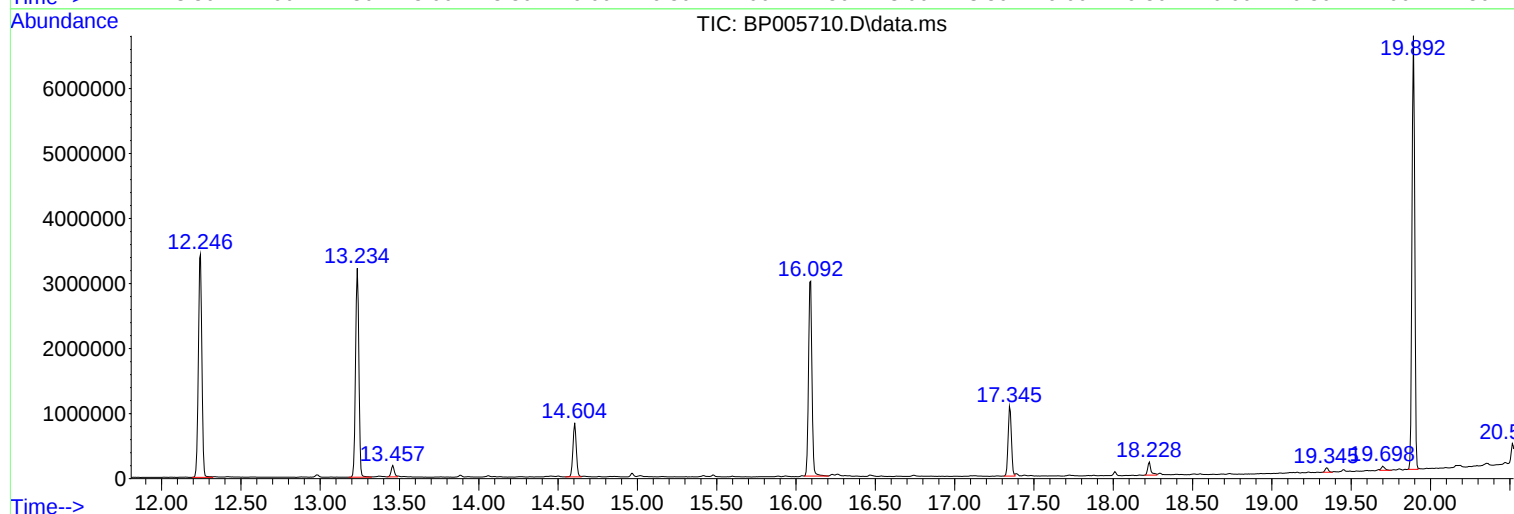
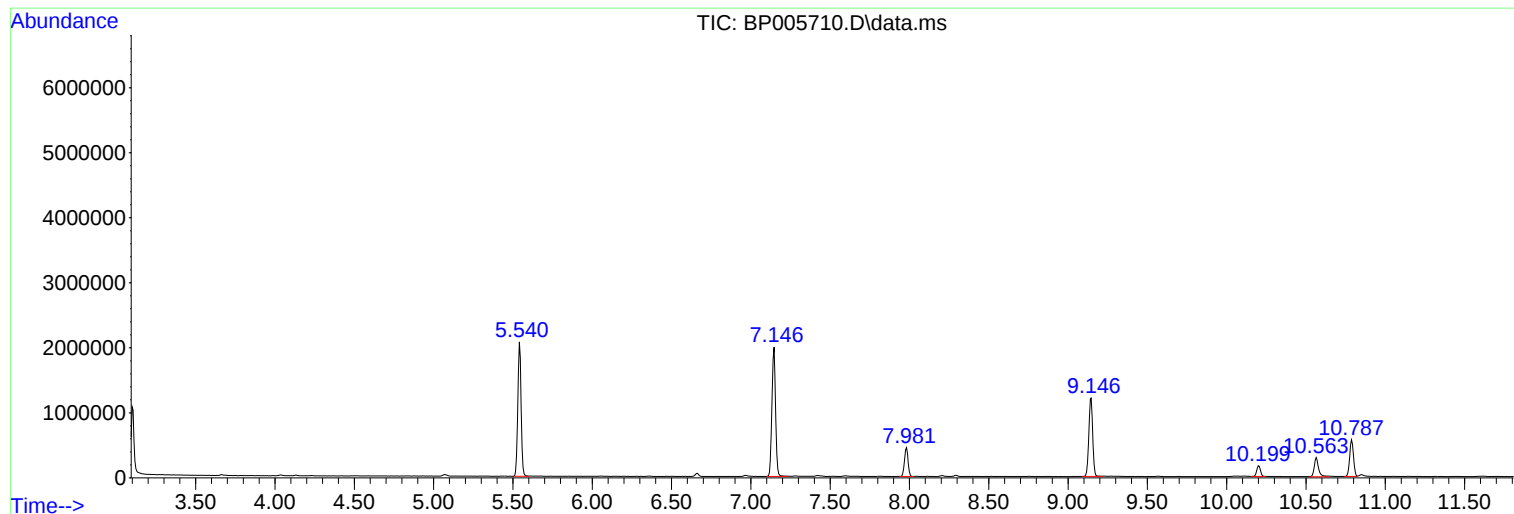
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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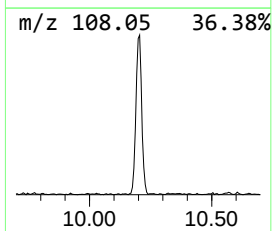
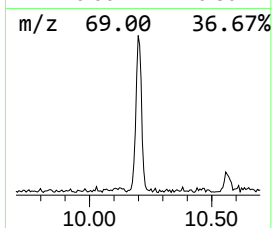
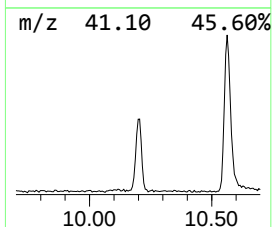
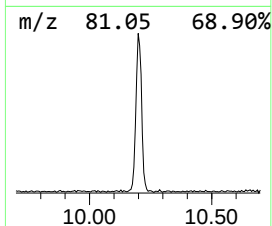
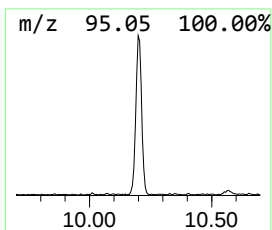
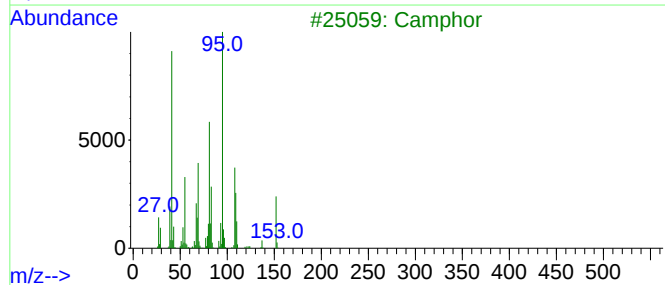
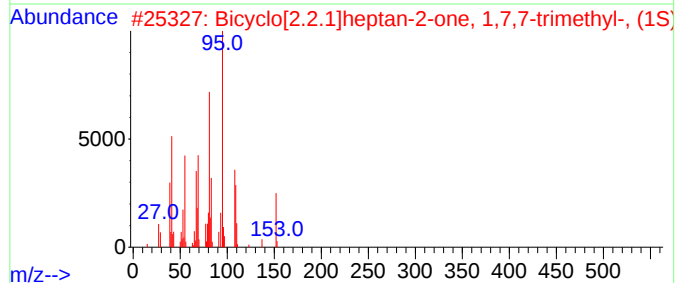
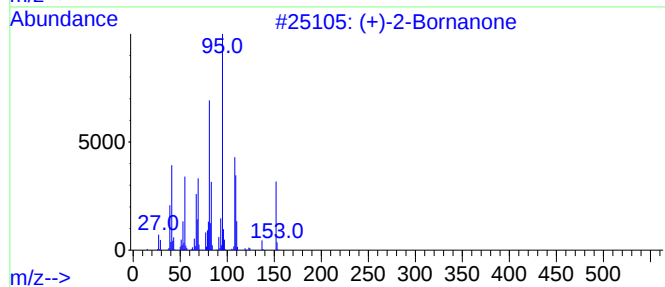
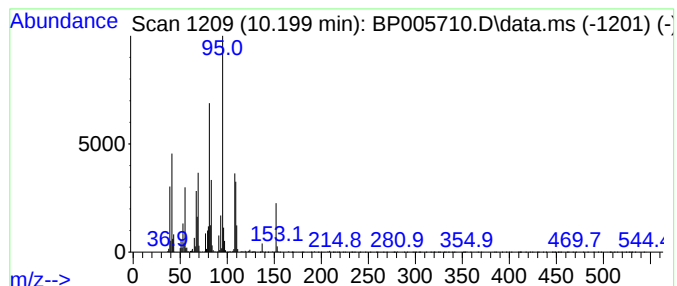
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (+)-2-Bornanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.199	5.85 ng	272502	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-2-Bornanone	152	C10H16O	000464-49-3	97
2			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
3			Camphor	152	C10H16O	000076-22-2	97
4			2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	52
5			Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	46



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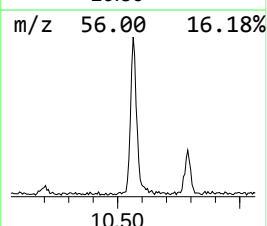
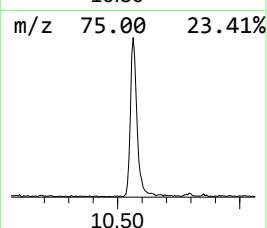
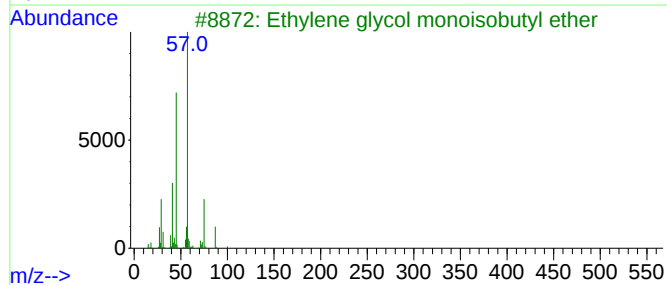
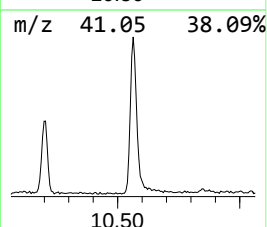
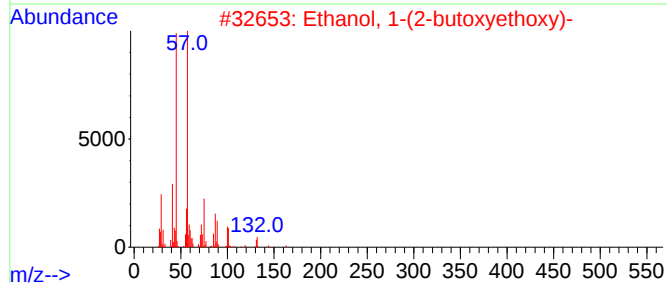
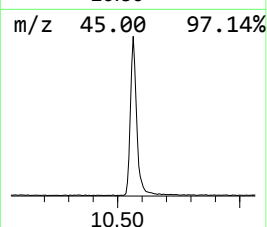
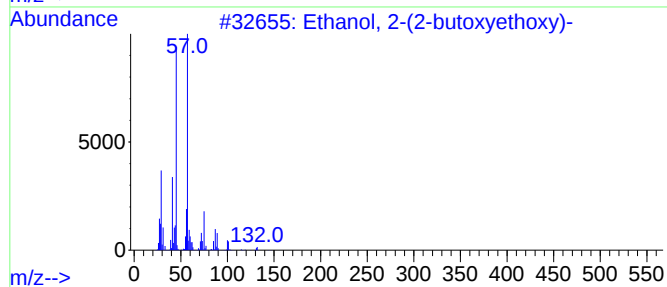
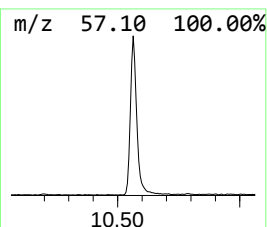
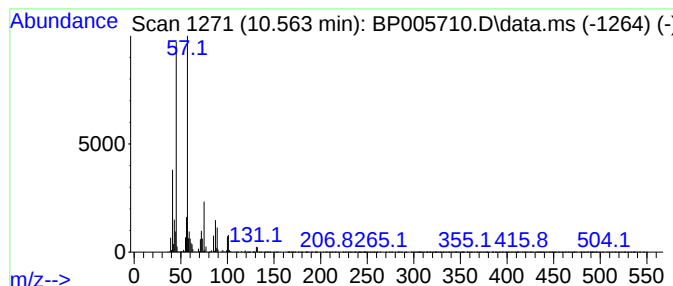
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.563	11.76 ng	547813	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	47
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	47



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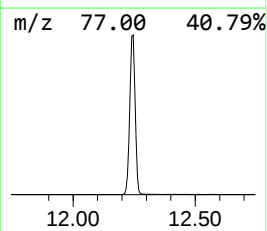
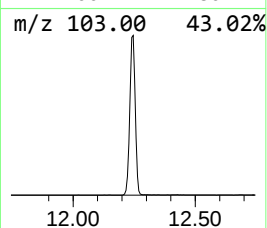
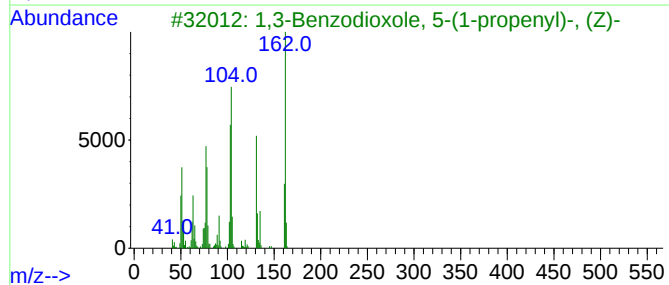
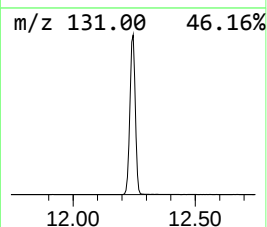
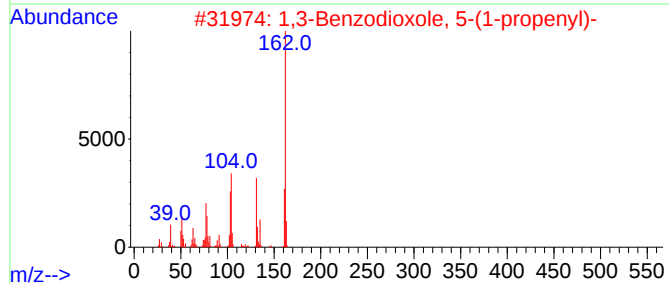
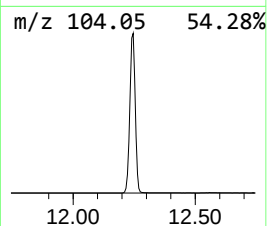
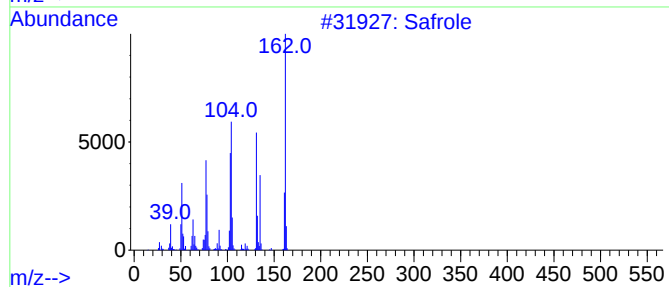
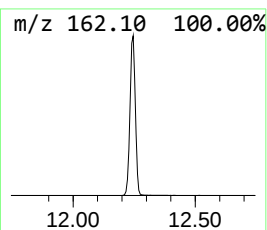
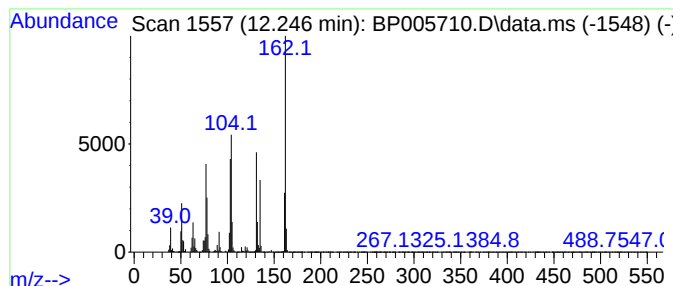
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Safrole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.246	114.08 ng	5314330	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Safrole	162	C10H10O2	000094-59-7	98
2			1,3-Benzodioxole, 5-(1-propenyl)-	162	C10H10O2	000120-58-1	97
3			1,3-Benzodioxole, 5-(1-propenyl)-...	162	C10H10O2	017627-76-8	97
4			Benzene, 1,2-(methylenedioxy)-4-...	162	C10H10O2	004043-71-4	95
5			1,4-Dioxo-1,2,3,4-tetrahydrophth...	162	C8H6N2O2	001445-69-8	41



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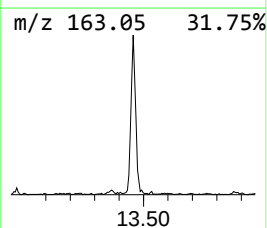
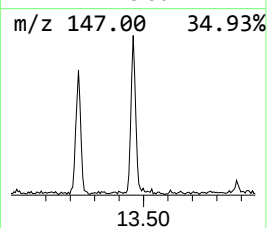
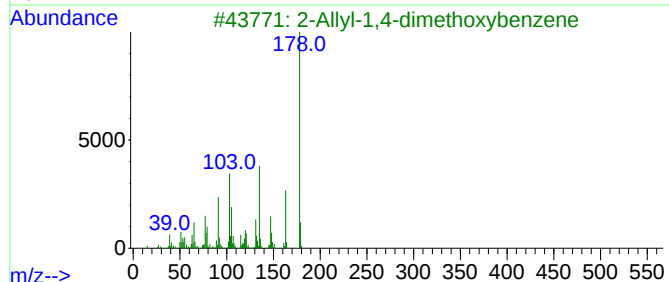
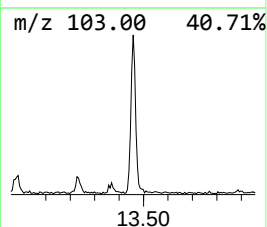
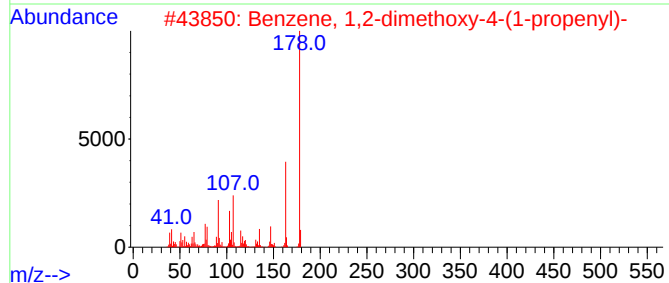
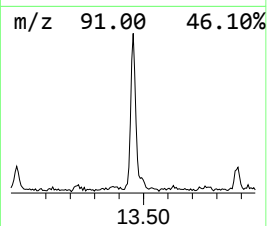
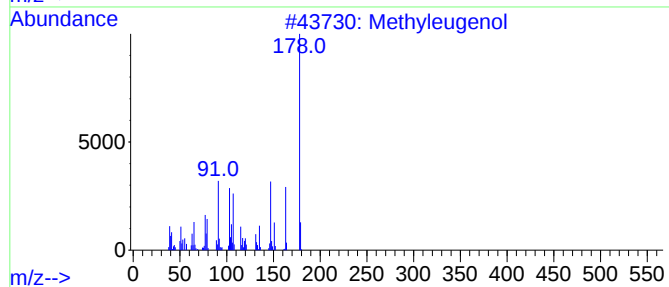
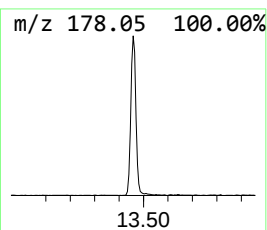
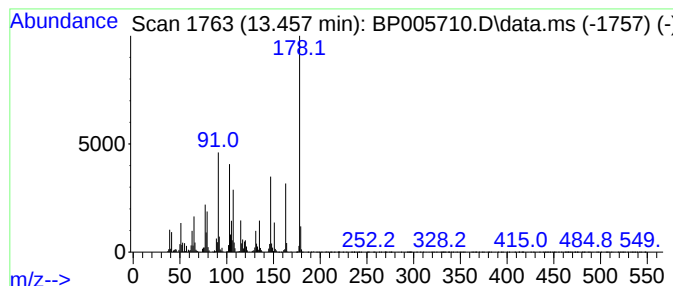
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Methyleugenol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.457	3.99 ng	244674	Acenaphthene-d10	14.604

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyleugenol	178	C11H14O2	000093-15-2	98
2			Benzene, 1,2-dimethoxy-4-(1-prop...	178	C11H14O2	000093-16-3	76
3			2-Allyl-1,4-dimethoxybenzene	178	C11H14O2	019754-22-4	52
4			4-Hydroxy-5-methyl-3-phenyl-.del...	178	C9H10N2O2	016227-04-6	38
5			7-Methoxy-3,4-dihydro-2[1H]-quin...	178	C9H10N2O2	055687-29-1	38



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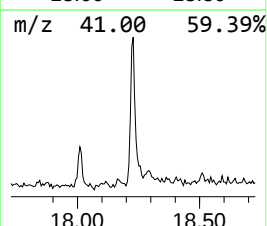
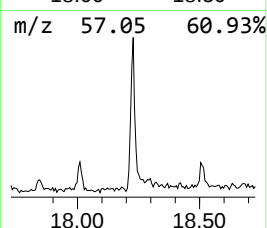
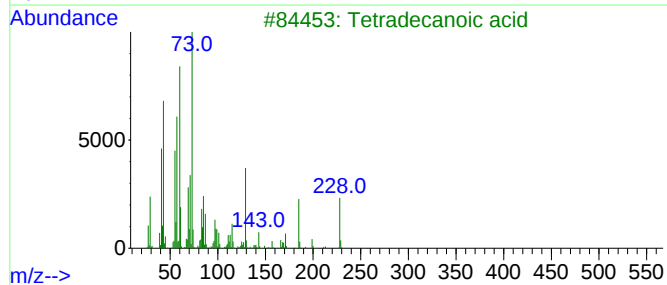
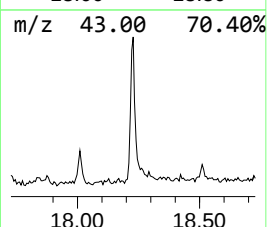
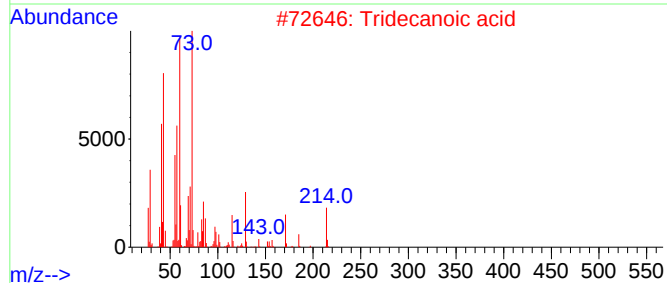
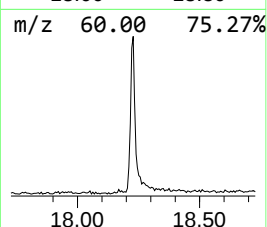
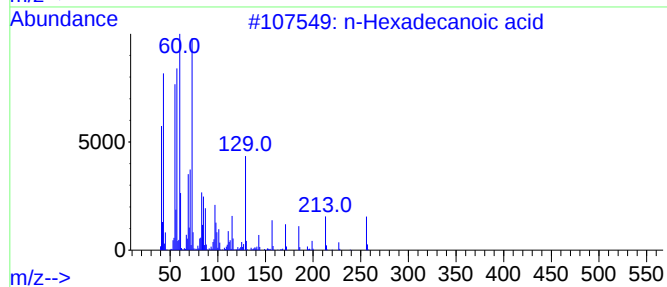
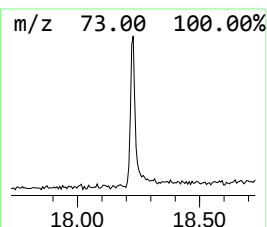
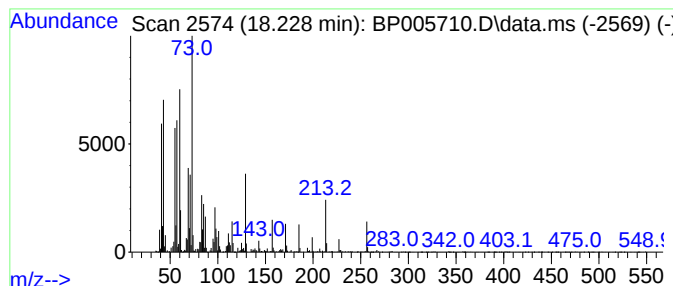
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.228	3.86 ng	295291	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



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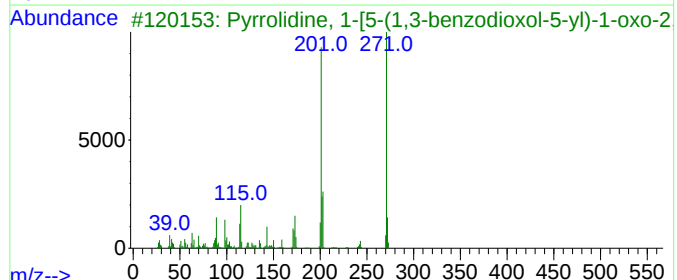
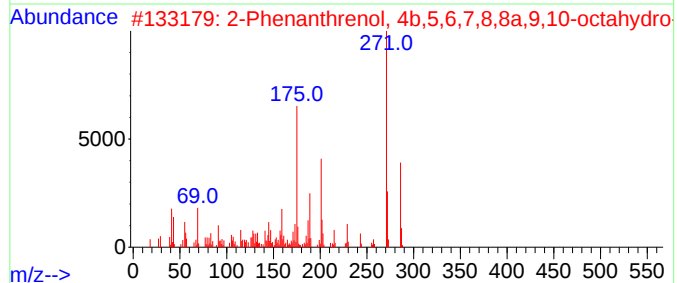
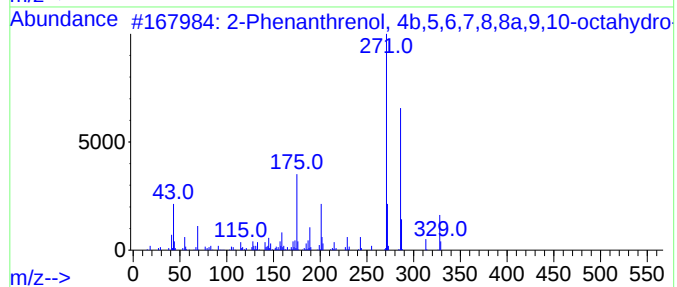
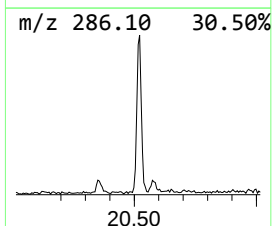
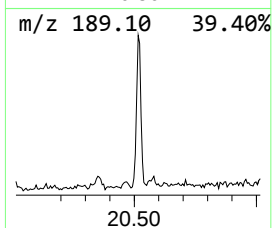
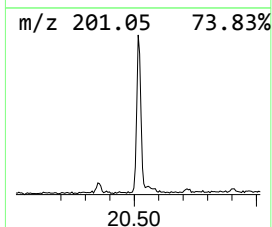
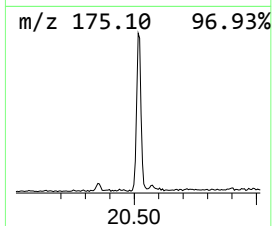
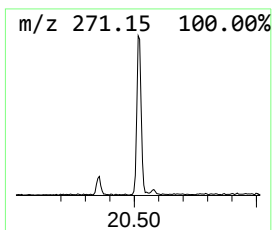
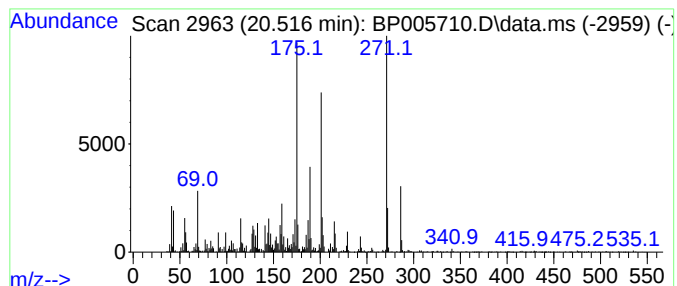
Instrument :
BNA_P
ClientSampleId :
T-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.516	3.71 ng	376025	Chrysene-d12	21.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	53
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	46
3	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	38
4	Podocarpa-8,11,13-trien-17-oic a...	344	C22H32O3	024067-43-4	38
5	Crinan-1-ol, 2,3-didehydro-, (1.a...	271	C16H17NO3	1000111-31-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060421\
Data File : BP005710.D
Acq On : 04 Jun 2021 13:37
Operator : CG/JU
Sample : M2611-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampled :
T-1

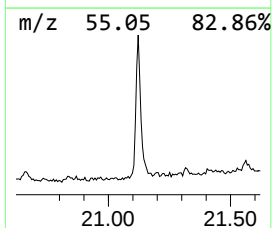
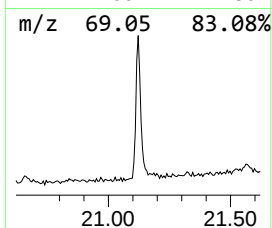
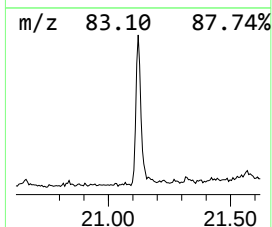
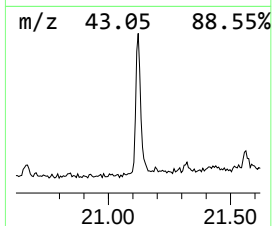
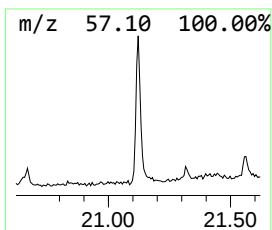
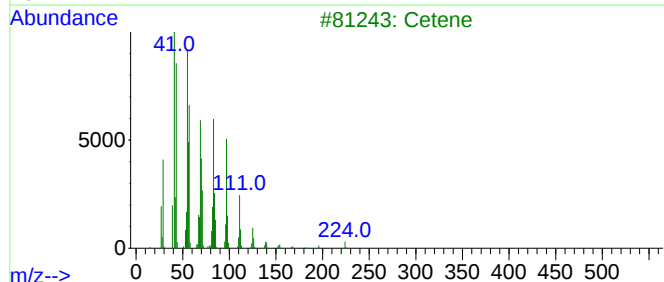
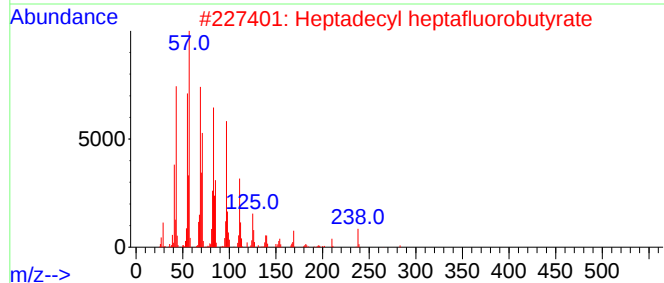
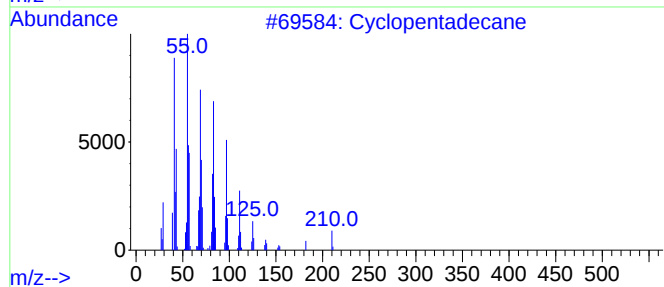
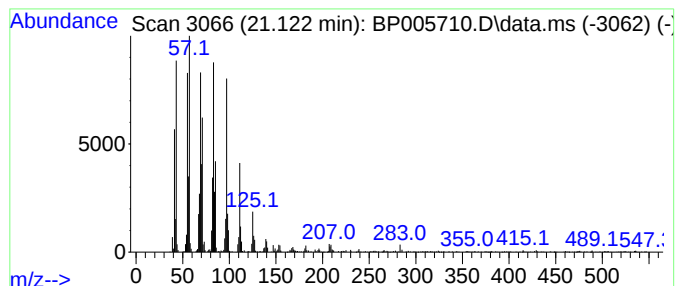
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.122	5.52 ng	559174	Chrysene-d12	21.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Cetene	224	C16H32	000629-73-2	92
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060421\
Data File : BP005710.D
Acq On : 04 Jun 2021 13:37
Operator : CG/JU
Sample : M2611-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
T-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.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-Bornanone	10.199	5.8	ng	272502	2	10.787	931703	20.0
Ethanol, 2-(2-b...	10.563	11.8	ng	547813	2	10.787	931703	20.0
Safrole	12.246	114.1	ng	5314330	2	10.787	931703	20.0
Methyleugenol	13.457	4.0	ng	244674	3	14.604	1227310	20.0
n-Hexadecanoic ...	18.228	3.9	ng	295291	4	17.345	1531210	20.0
2-Phenanthrenol...	20.516	3.7	ng	376025	5	21.416	2025880	20.0
Cyclopentadecane	21.122	5.5	ng	559174	5	21.416	2025880	20.0