

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
 Data File : BP005269.D
 Acq On : 12 Apr 2021 16:51
 Operator : CG/JU
 Sample : M1967-07
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SB2-B

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-BP040921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.822	290	295	305	rVB	694893	953773	81.71%	12.246%
2	5.275	368	372	380	rVB	146883	224507	19.23%	2.883%
3	6.864	636	642	660	rVB2	395246	874005	74.87%	11.222%
4	7.675	774	780	787	rVV	127521	200197	17.15%	2.571%
5	7.740	788	791	797	rVB2	10224	15885	1.36%	0.204%
6	8.840	971	978	985	rBV	263574	435967	37.35%	5.598%
7	9.240	1037	1046	1051	rVB4	6909	12237	1.05%	0.157%
8	10.463	1247	1254	1260	rBV	137813	236237	20.24%	3.033%
9	11.981	1507	1512	1520	rBV2	21616	39988	3.43%	0.513%
10	12.951	1666	1677	1684	rBV	515964	716209	61.35%	9.196%
11	13.798	1816	1821	1829	rVV	20604	33724	2.89%	0.433%
12	14.063	1862	1866	1872	rBV6	6642	11833	1.01%	0.152%
13	14.340	1907	1913	1921	rVB	210461	299444	25.65%	3.845%
14	16.087	2203	2210	2215	rBV8	7473	17939	1.54%	0.230%
15	16.498	2278	2280	2287	rVB8	7372	12957	1.11%	0.166%
16	17.104	2377	2383	2387	rBV	262965	377942	32.38%	4.853%
17	17.145	2387	2390	2395	rVB	23219	26613	2.28%	0.342%
18	17.198	2395	2399	2402	rBV	46240	51317	4.40%	0.659%
19	18.163	2561	2563	2568	rVB5	11764	14491	1.24%	0.186%
20	18.992	2700	2704	2712	rBV2	78567	129749	11.12%	1.666%
21	19.128	2723	2727	2731	rVB	76318	93345	8.00%	1.199%
22	19.181	2733	2736	2741	rVB7	12382	16209	1.39%	0.208%
23	19.481	2783	2787	2789	rBV	61457	76439	6.55%	0.981%
24	19.681	2816	2821	2826	rBV	1037834	1167330	100.00%	14.989%
25	20.922	3028	3032	3039	rVB2	122248	256160	21.94%	3.289%
26	20.986	3039	3043	3050	rVB	242225	299495	25.66%	3.846%
27	21.116	3062	3065	3069	rVB	63434	70451	6.04%	0.905%
28	21.204	3075	3080	3084	rBV	426126	560925	48.05%	7.202%
29	22.774	3344	3347	3352	rBV4	66588	111177	9.52%	1.428%
30	23.474	3461	3466	3476	rVB2	242443	451604	38.69%	5.799%

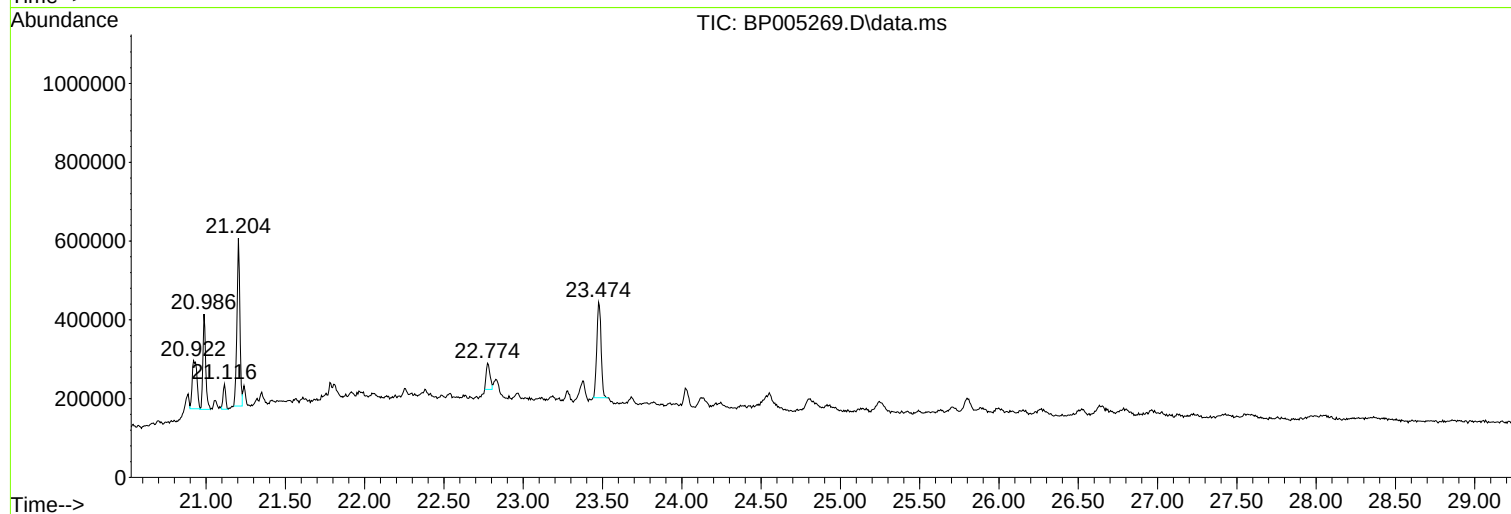
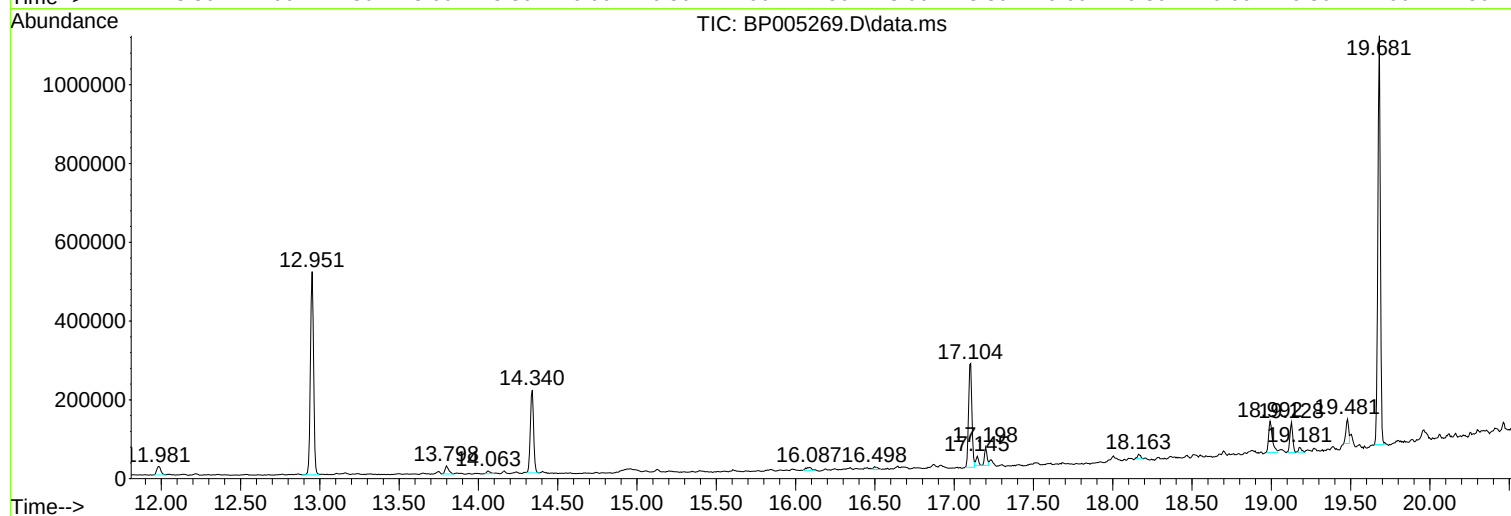
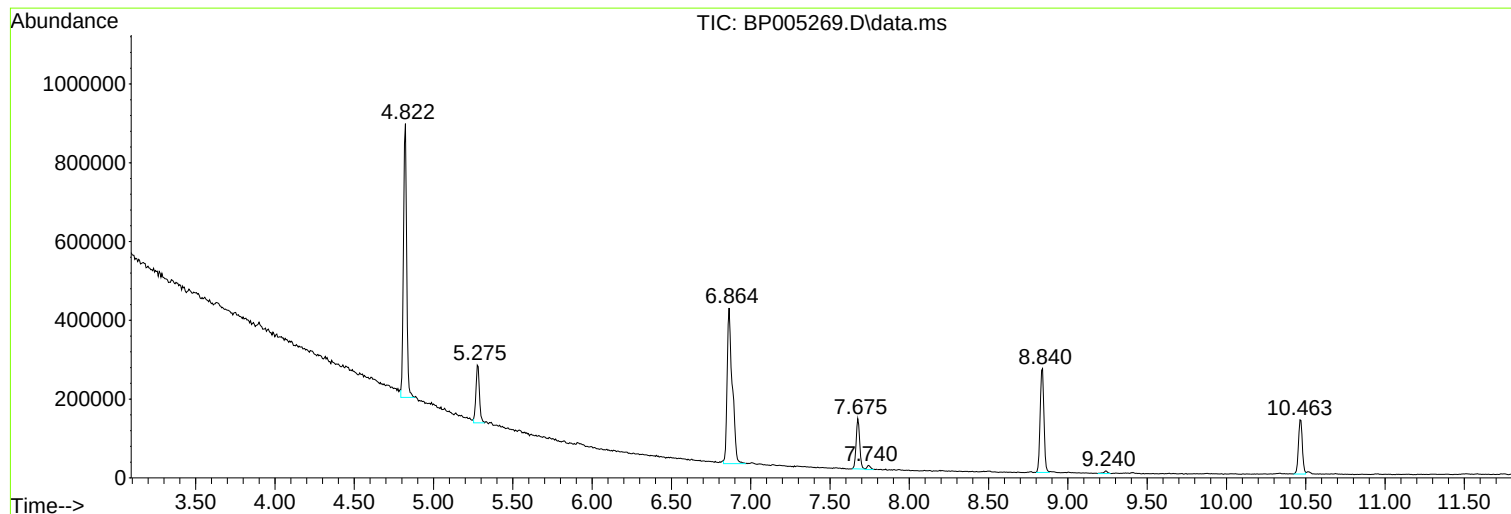
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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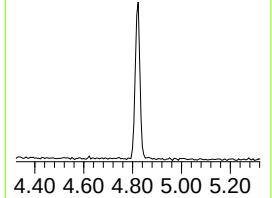
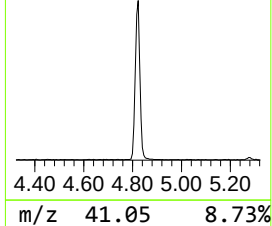
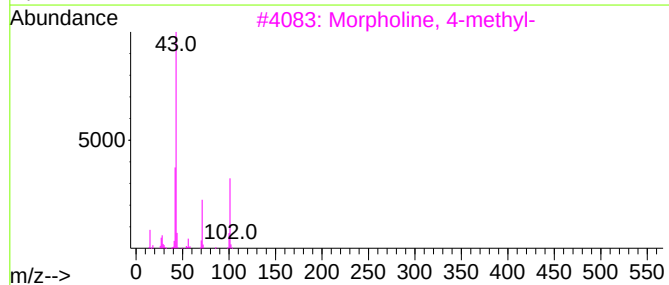
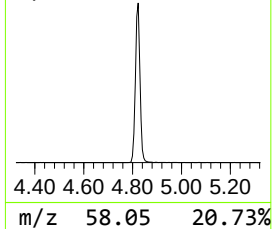
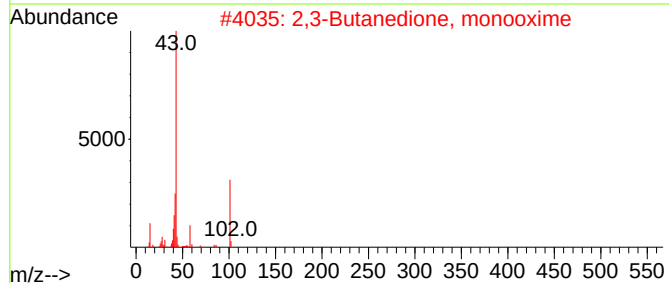
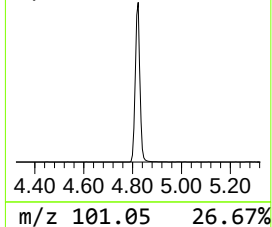
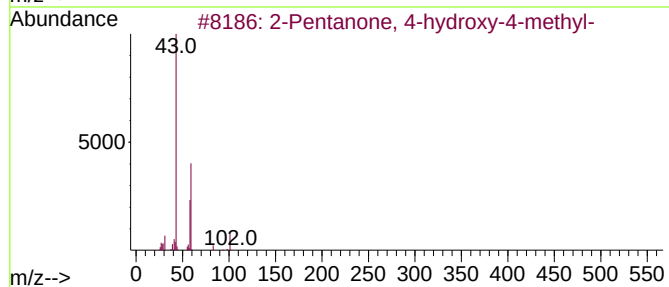
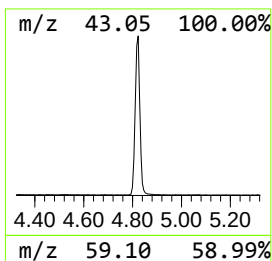
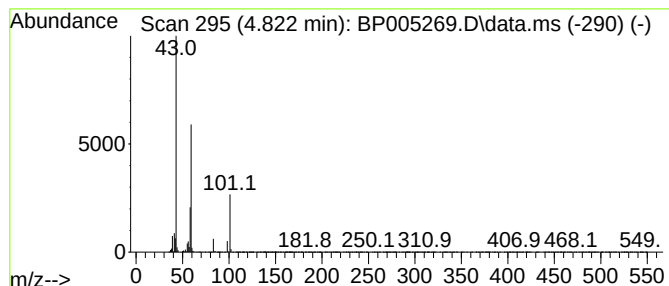
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.822	95.28 ng	953773	1,4-Dichlorobenzene-d4	7.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9		
5	Acetone	58	C3H6O	000067-64-1	9		



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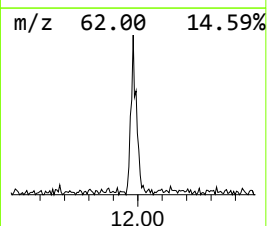
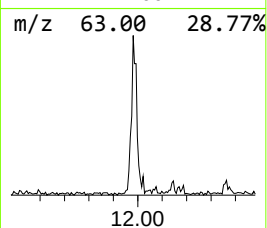
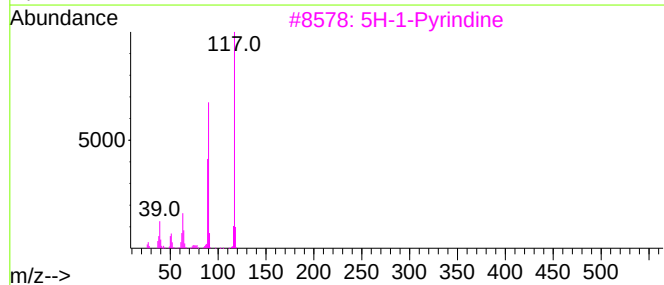
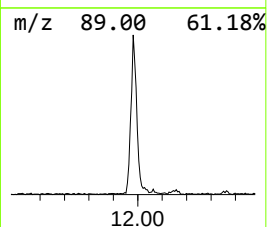
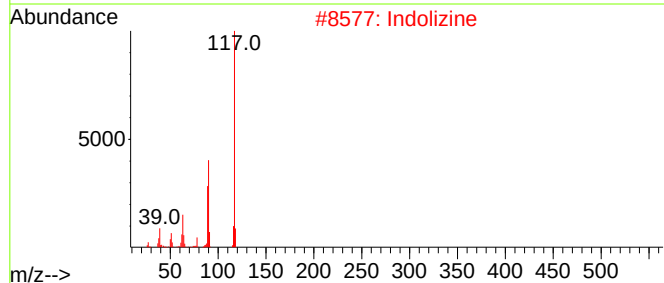
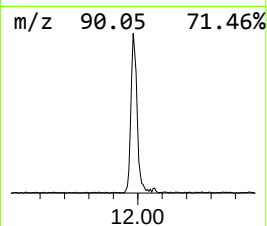
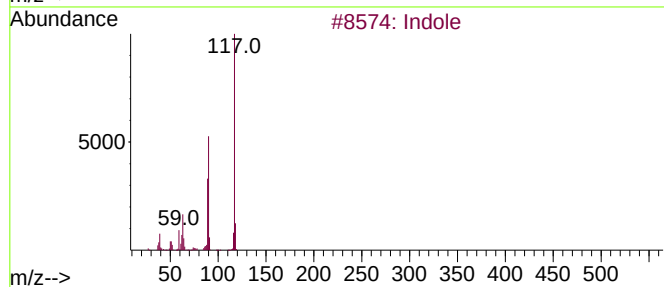
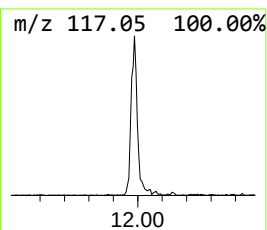
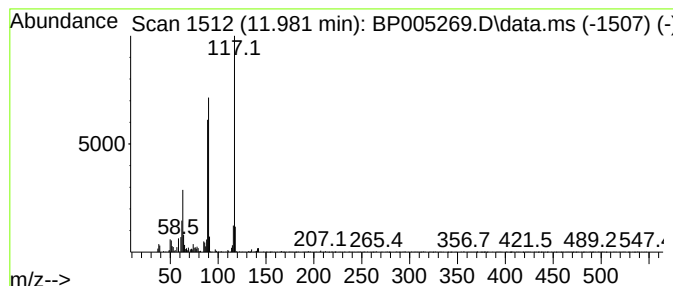
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Peak Number 2 Indole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.981	3.39 ng	39988	Naphthalene-d8	10.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	94
2			Indolizine	117	C8H7N	000274-40-8	91
3			5H-1-Pyridine	117	C8H7N	000270-91-7	91
4			Benzyl nitrile	117	C8H7N	000140-29-4	83
5			1H-Indole-1-carboxaldehyde, 2,3-...	163	C9H9NO2	013303-68-9	83



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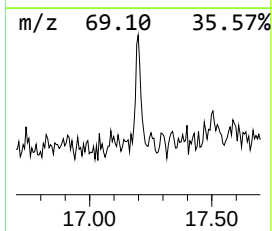
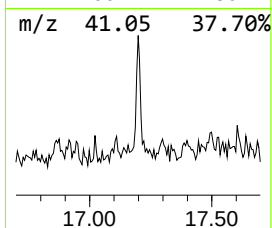
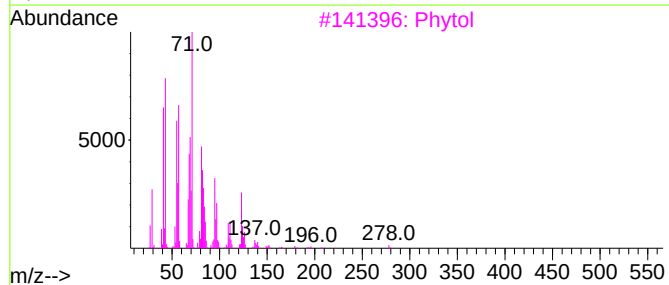
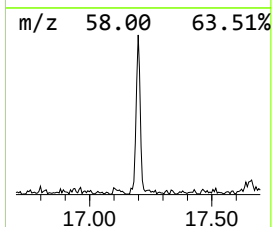
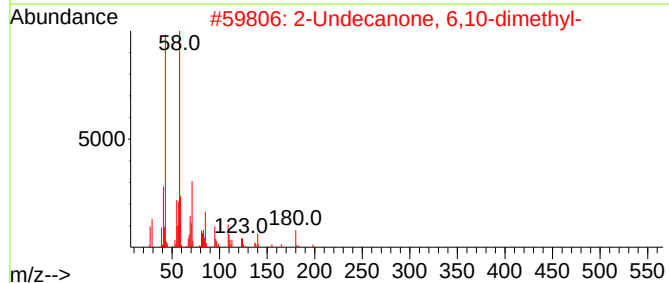
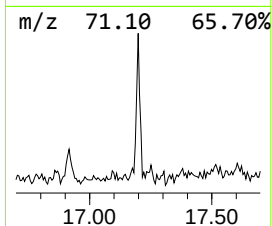
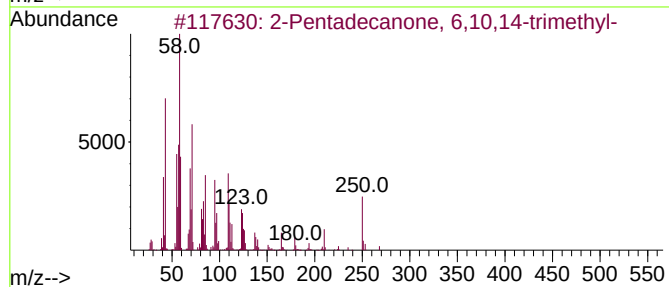
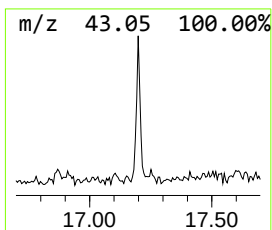
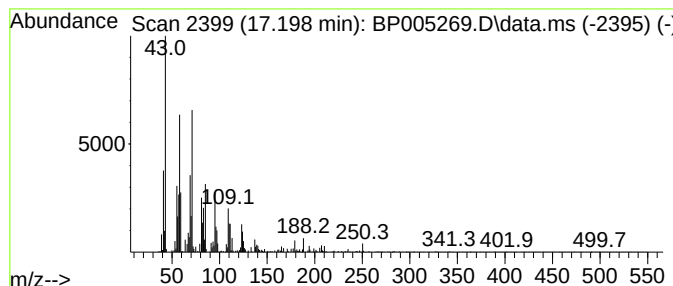
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 2-Pentadecanone, 6,10,14-tr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.198	2.72 ng	51317	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentadecanone, 6,10,14-trimethyl-	268	C18H36O	000502-69-2	58		
2	2-Undecanone, 6,10-dimethyl-	198	C13H26O	001604-34-8	53		
3	Phytol	296	C20H40O	000150-86-7	46		
4	Octadecanal	268	C18H36O	000638-66-4	35		
5	2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	35		



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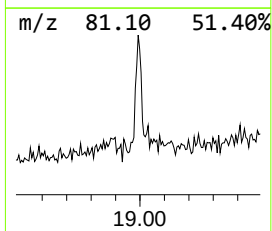
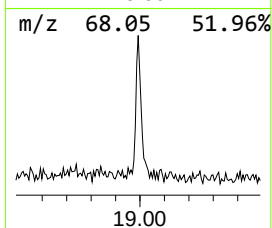
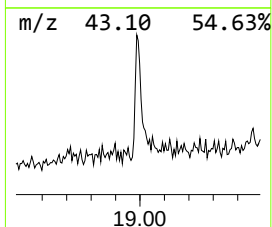
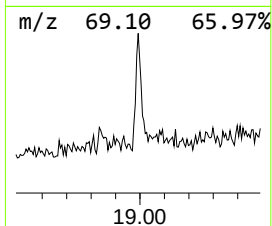
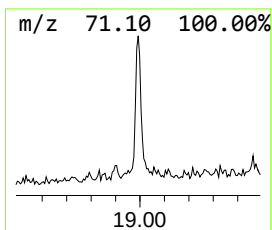
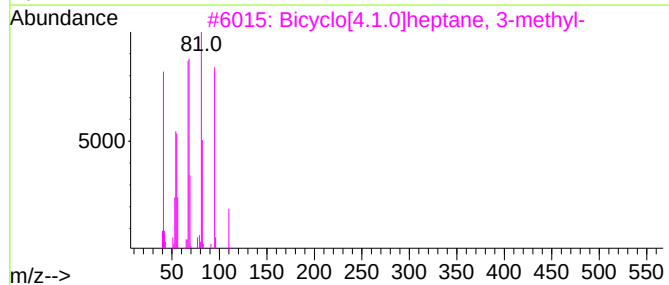
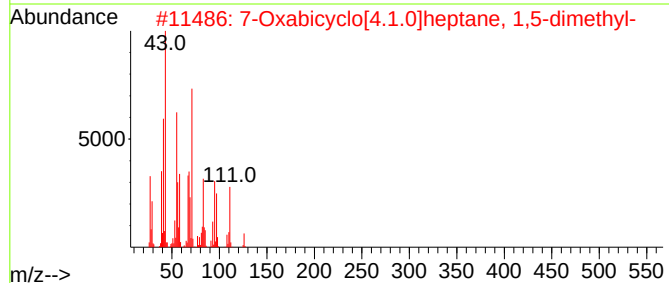
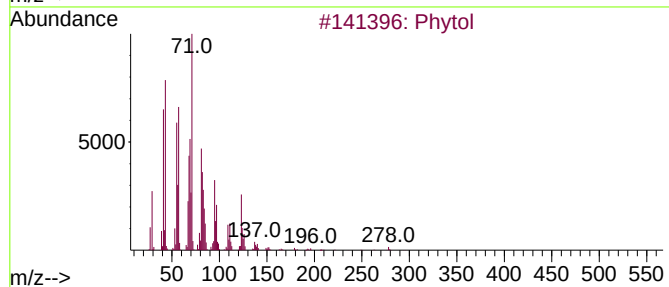
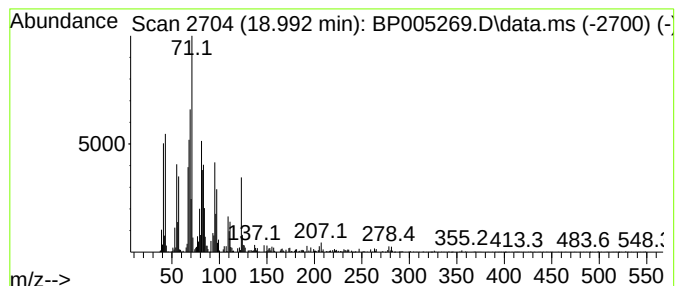
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Peak Number 4 Phytol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.992	6.87 ng	129749	Phenanthrene-d10	17.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phytol	296	C20H40O	000150-86-7	93
2			7-Oxabicyclo[4.1.0]heptane, 1,5-...	126	C8H14O	162239-52-3	80
3			Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	42
4			2-Isopropenyl-5-methyl-6-hepten-...	168	C11H20O	013066-55-2	38
5			3,7,11,15-Tetramethyl-2-hexadec...	296	C20H40O	102608-53-7	35



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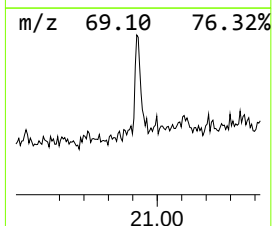
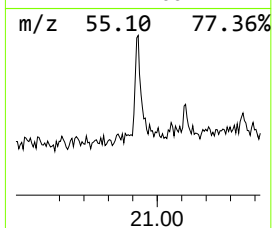
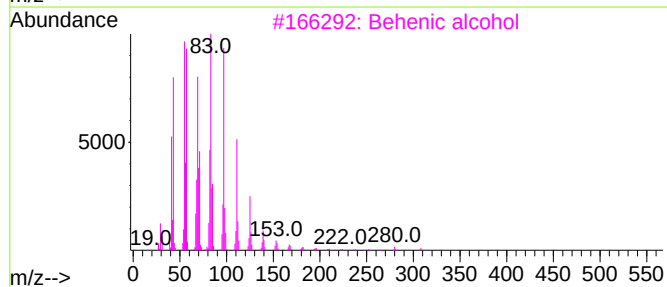
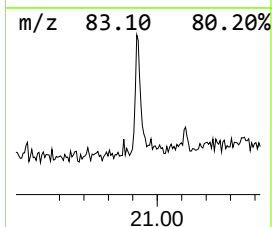
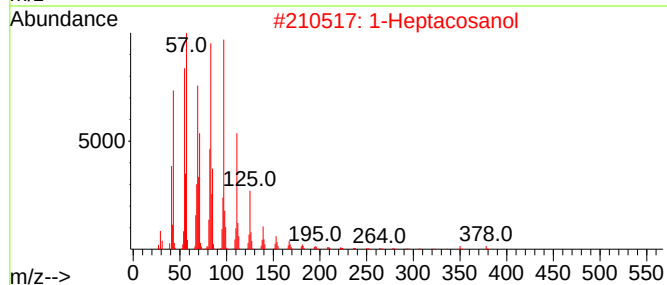
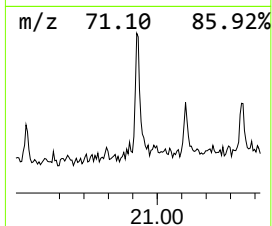
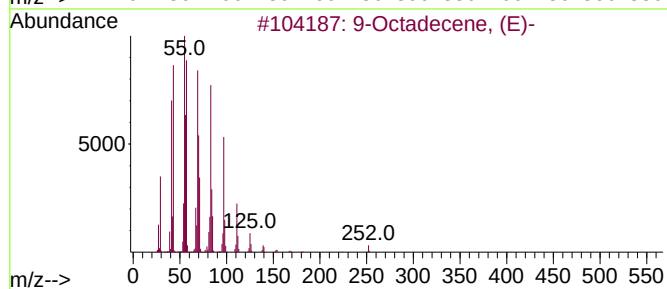
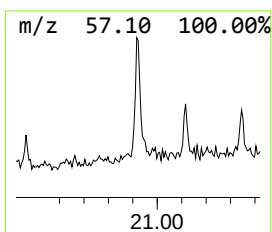
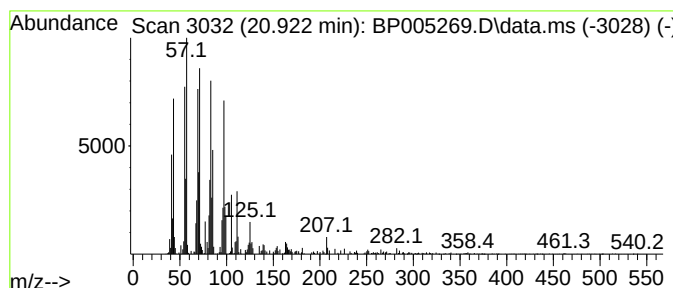
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 9-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.922	9.13 ng	256160	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecene, (E)-	252	C18H36	007206-25-9	86
2			1-Heptacosanol	396	C27H56O	002004-39-9	81
3			Behenic alcohol	326	C22H46O	000661-19-8	76
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	76
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	76



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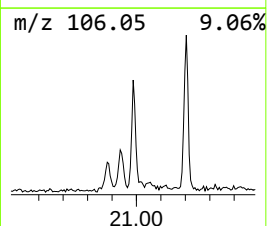
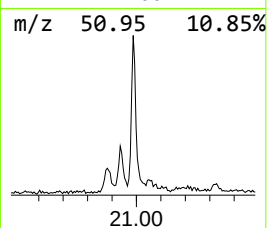
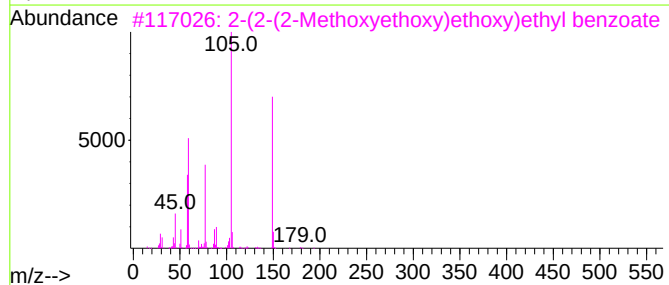
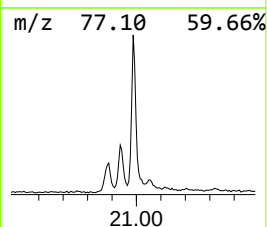
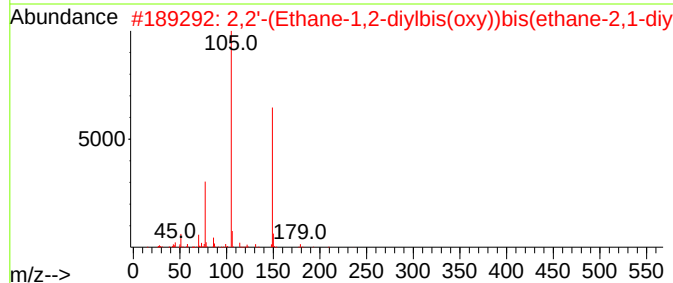
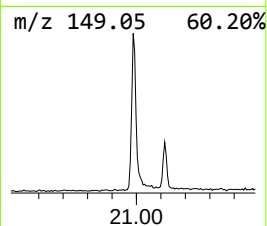
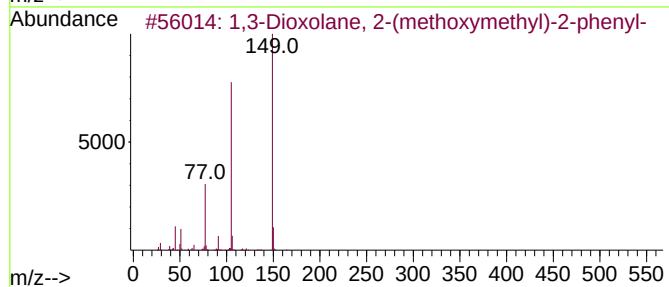
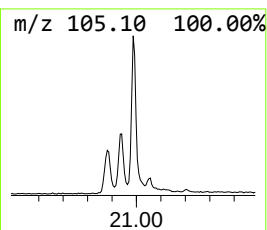
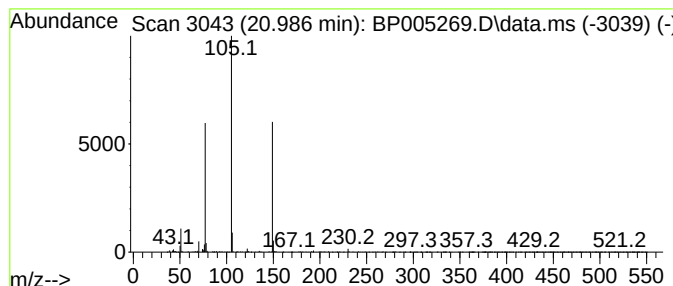
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.986	10.68 ng	299495	Chrysene-d12	21.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	56
3			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	50
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP041221\
Data File : BP005269.D
Acq On : 12 Apr 2021 16:51
Operator : CG/JU
Sample : M1967-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB2-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP040921.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-...	4.822	95.3	ng	953773	1	7.675	200197	20.0
Indole	11.981	3.4	ng	39988	2	10.463	236237	20.0
2-Pentadecanone...	17.198	2.7	ng	51317	4	17.104	377942	20.0
Phytol	18.992	6.9	ng	129749	4	17.104	377942	20.0
9-Octadecene, (E)-	20.922	9.1	ng	256160	5	21.204	560925	20.0
1,3-Dioxolane, ...	20.986	10.7	ng	299495	5	21.204	560925	20.0