

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
 Data File : BF131575.D
 Acq On : 09 Dec 2022 19:45
 Operator : CG\JU
 Sample : N5963-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBR200014-RB21197

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_F\Methods\8270-BF120822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131575.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	17	26	32	rVB	582601	734391	24.47%	3.848%
2	5.140	514	519	530	rVB	213992	314169	10.47%	1.646%
3	5.528	579	585	588	rBV	2242996	2276084	75.85%	11.927%
4	6.534	749	756	759	rBV	2093938	2375049	79.14%	12.446%
5	6.904	816	819	823	rBV	470714	405561	13.51%	2.125%
6	7.475	910	916	919	rBV	1384068	1528932	50.95%	8.012%
7	8.198	1034	1039	1042	rBV	501758	508114	16.93%	2.663%
8	9.281	1216	1223	1226	rBV	3193888	2948005	98.24%	15.448%
9	9.610	1276	1279	1284	rVB3	96031	80439	2.68%	0.422%
10	9.957	1333	1338	1342	rVB	663748	654312	21.80%	3.429%
11	10.475	1419	1426	1430	rVB	123006	116995	3.90%	0.613%
12	10.757	1467	1474	1477	rBV	2290920	2109826	70.31%	11.056%
13	11.451	1588	1592	1595	rBV	767009	653553	21.78%	3.425%
14	11.974	1678	1681	1685	rBV	66772	54445	1.81%	0.285%
15	12.010	1685	1687	1691	rVB	40895	33654	1.12%	0.176%
16	13.051	1859	1864	1867	rBV	3415477	3000891	100.00%	15.725%
17	14.016	2021	2028	2029	rBV3	21990	38293	1.28%	0.201%
18	14.104	2039	2043	2051	rVB	546473	475233	15.84%	2.490%
19	14.198	2053	2059	2066	rVB	297410	298928	9.96%	1.566%
20	14.968	2186	2190	2195	rVB	87000	88564	2.95%	0.464%
21	15.615	2295	2300	2309	rBV	293903	353641	11.78%	1.853%
22	16.104	2378	2383	2392	rBV2	19661	33901	1.13%	0.178%

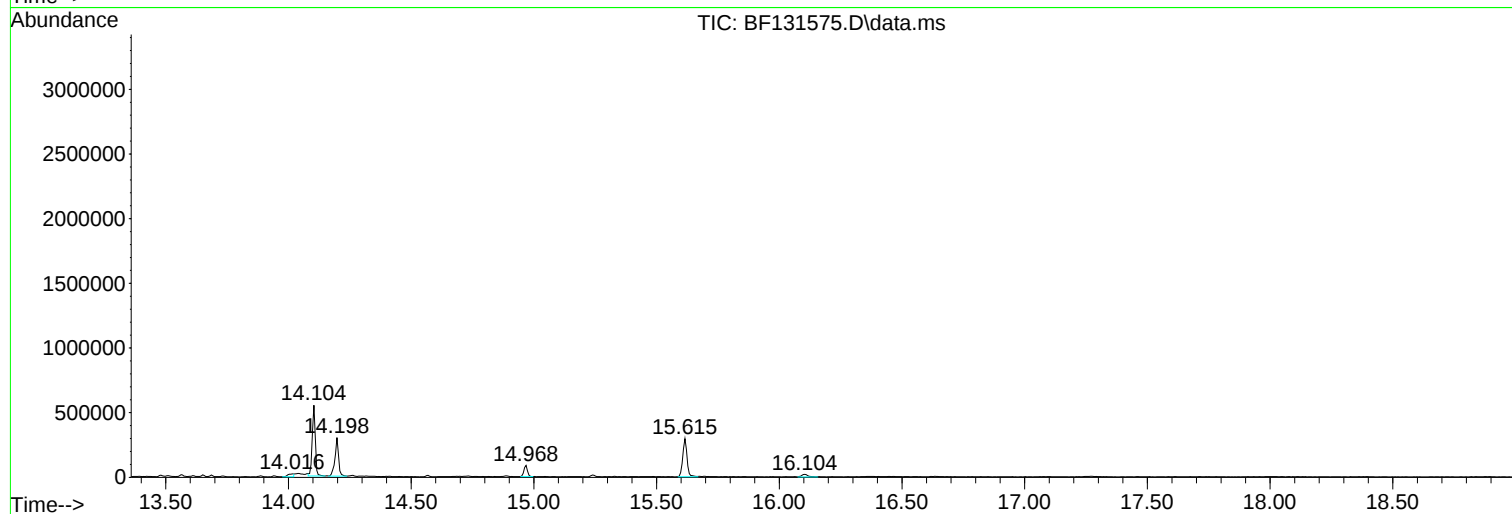
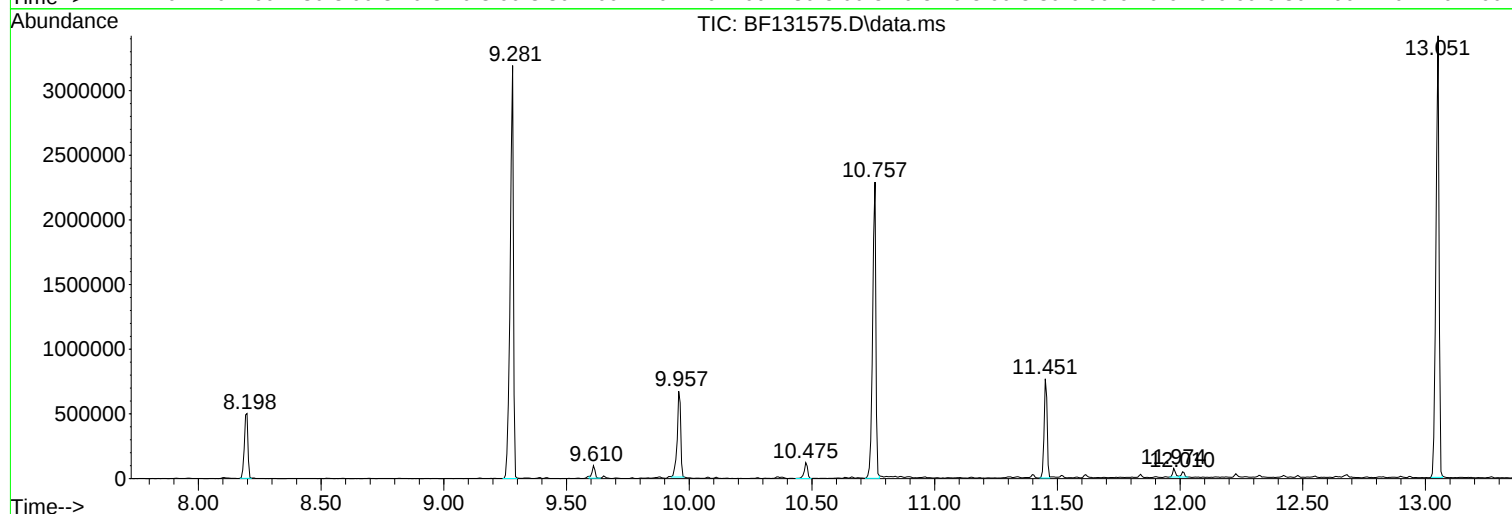
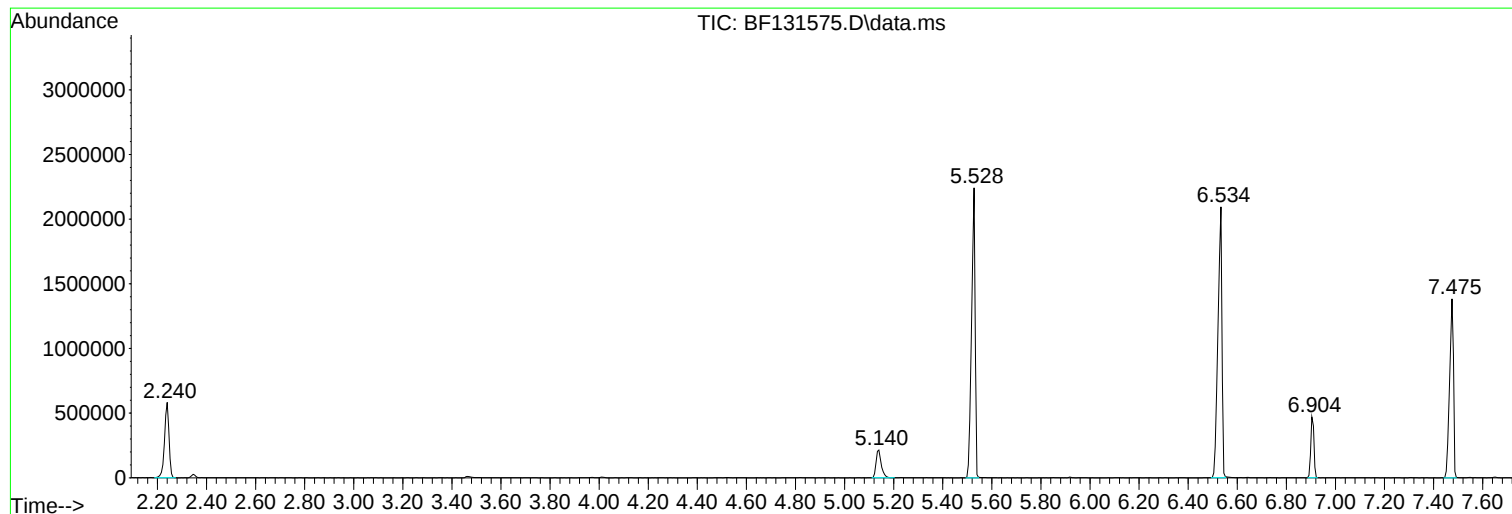
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ClientSampleId :
RBR200014-RB21197

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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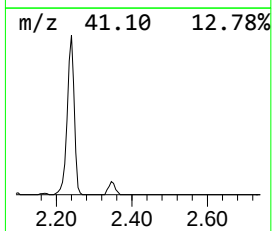
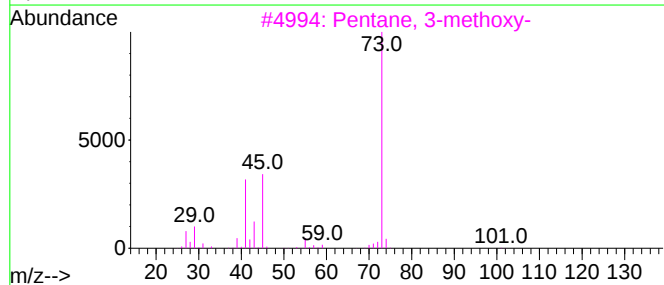
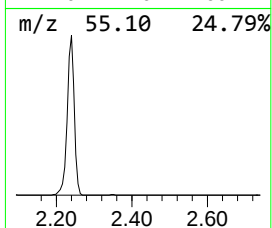
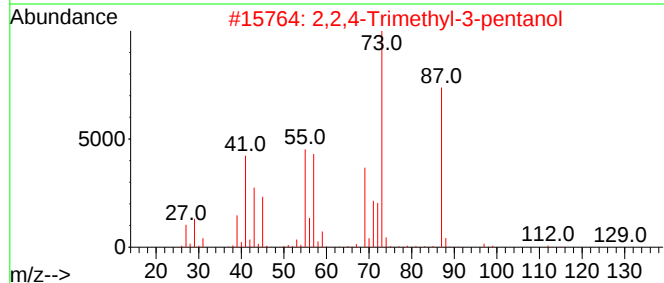
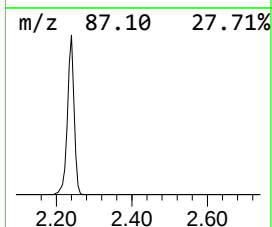
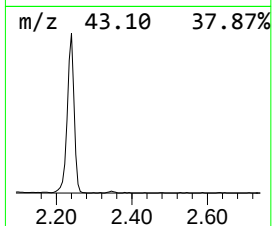
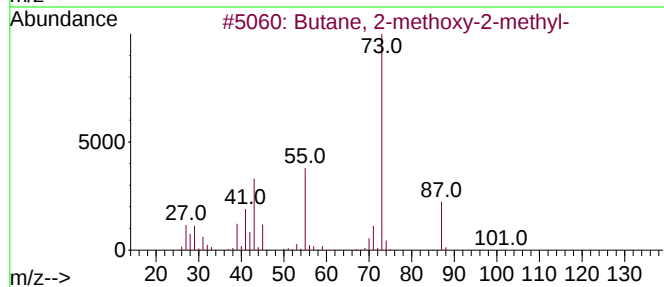
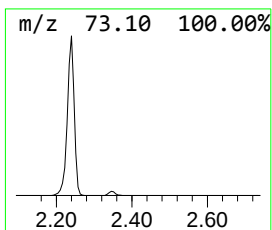
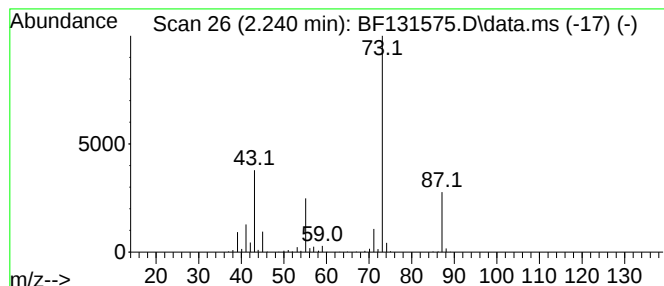
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	36.22 ng	734391	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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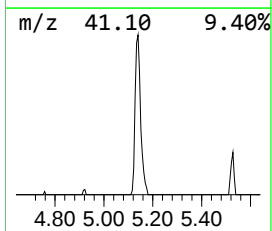
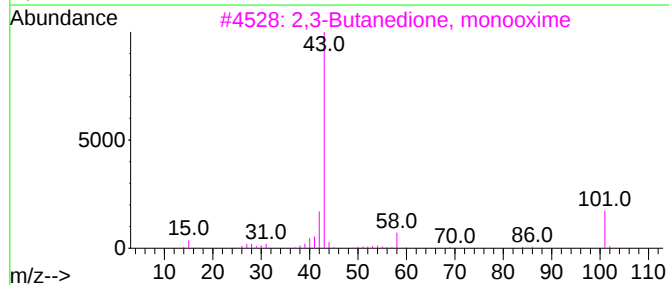
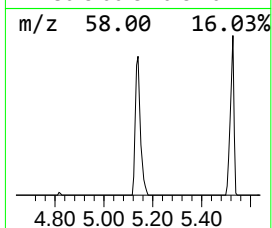
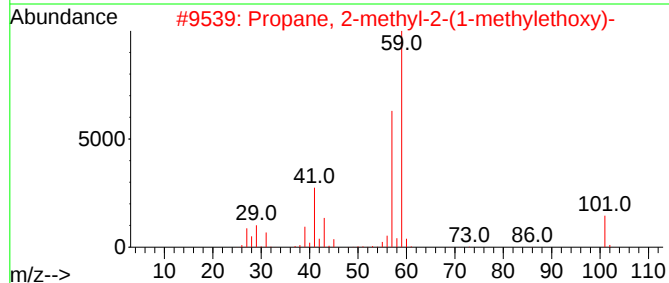
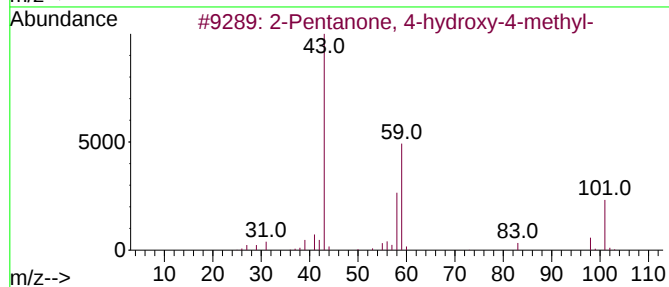
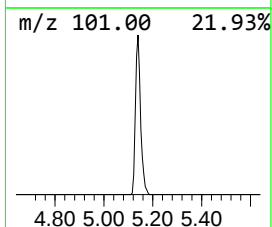
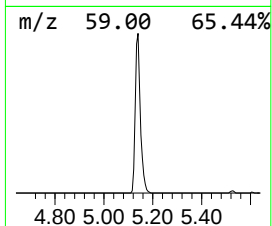
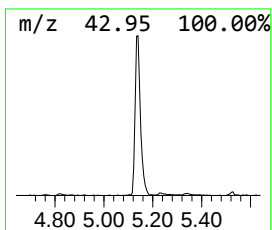
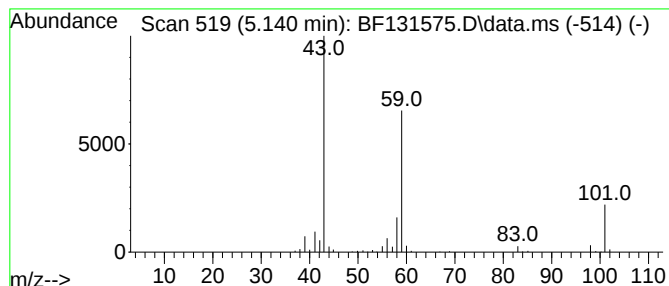
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.140	15.49 ng	314169	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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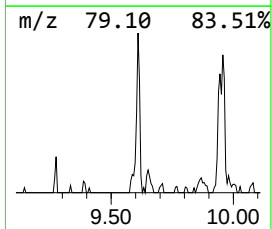
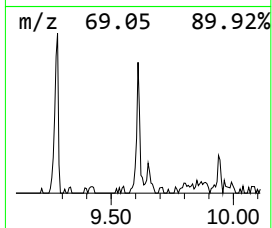
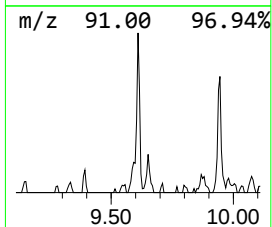
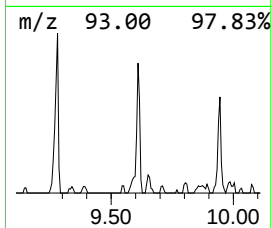
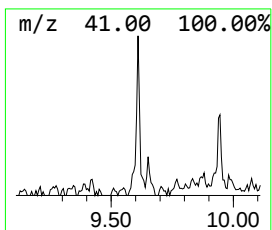
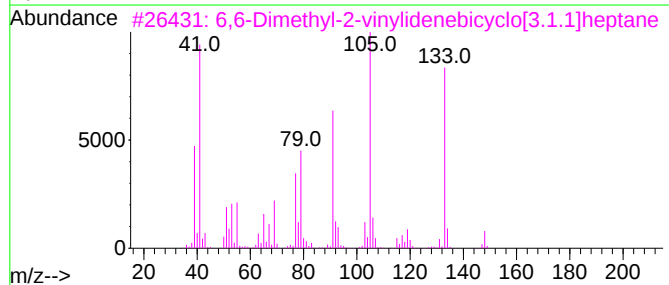
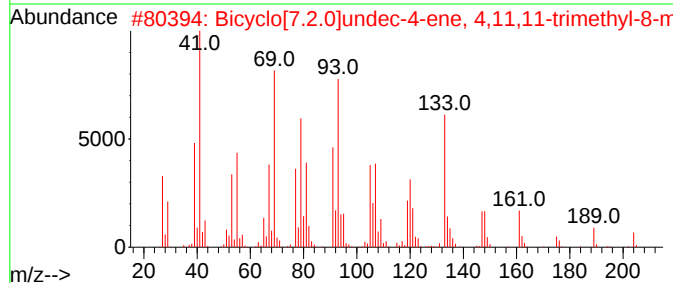
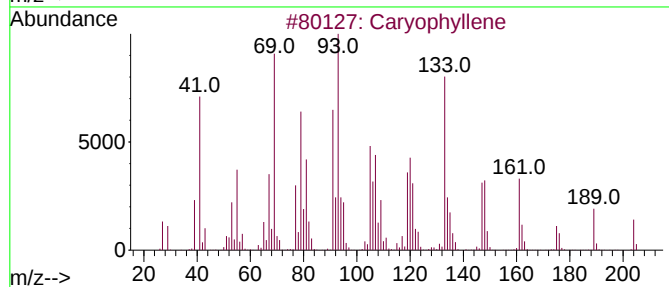
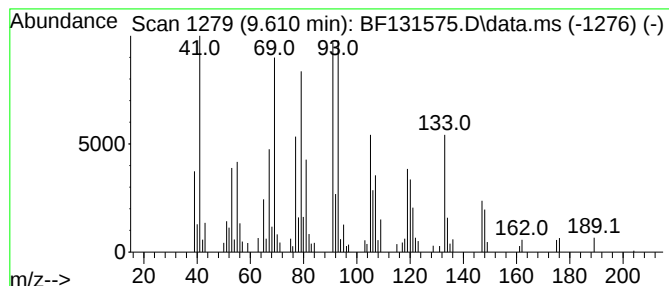
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Caryophyllene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.610	2.46 ng	80439	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Caryophyllene	204	C15H24	000087-44-5	53
2			Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	49
3			6,6-Dimethyl-2-vinylidenebicyclo...	148	C11H16	039021-75-5	38
4			(2R,4R)-p-Mentha-[1(7),8]-diene,...	168	C10H16O2	1000292-74-1	35
5			1,7-Octadiene, 2,7-dimethyl-3,6-...	162	C12H18	016714-60-6	35



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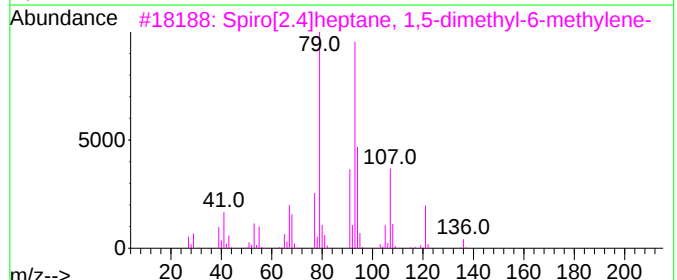
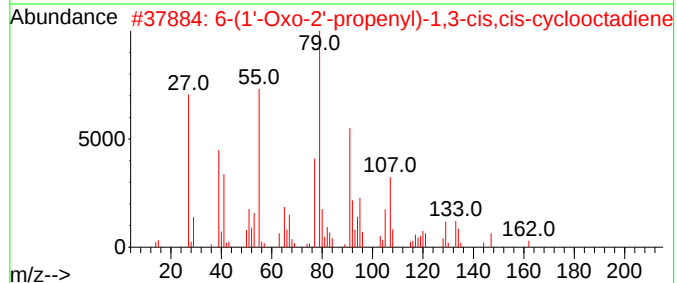
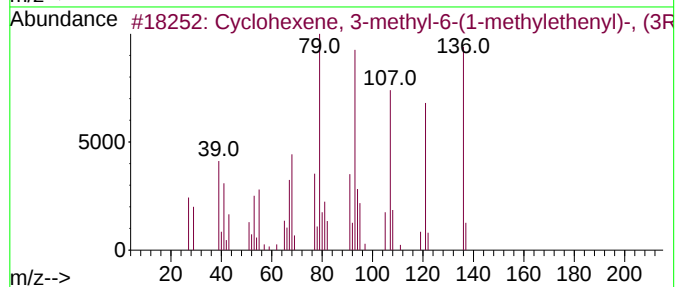
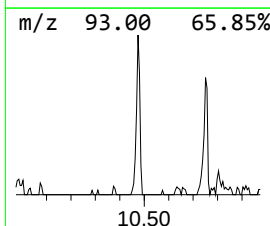
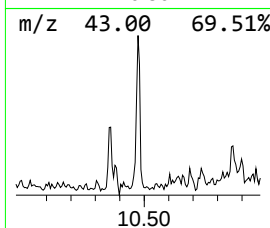
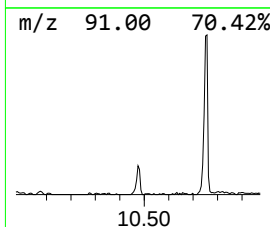
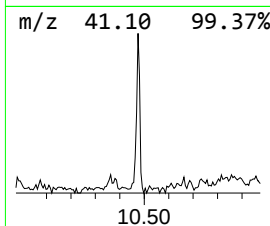
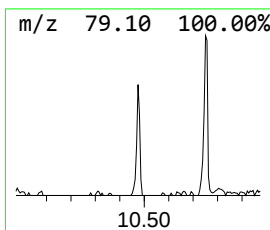
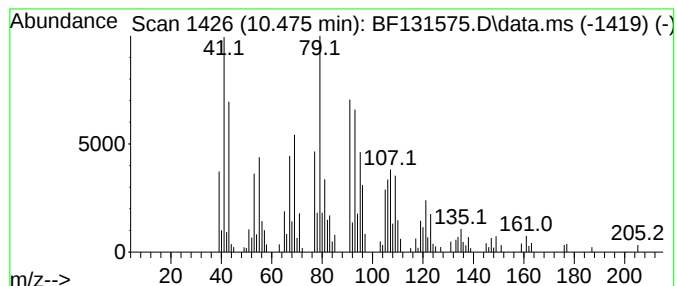
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Peak Number 4 Cyclohexene, 3-methyl-6-(1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.475	3.58 ng	116995	Acenaphthene-d10	9.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	005113-87-1	60
2			6-(1'-Oxo-2'-propenyl)-1,3-cis,c...	162	C11H14O	138146-05-1	43
3			Spiro[2.4]heptane, 1,5-dimethyl-...	136	C10H16	062238-24-8	38
4			Cyclohexene, 4-methyl-1-(1-methy...	136	C10H16	000586-67-4	38
5			Bicyclo[2.2.1]hepta-2,5-dien-7-ol	108	C7H8O	000822-80-0	35



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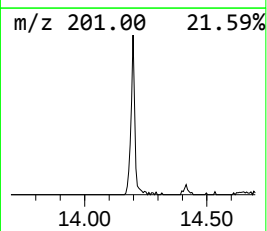
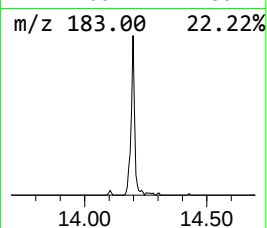
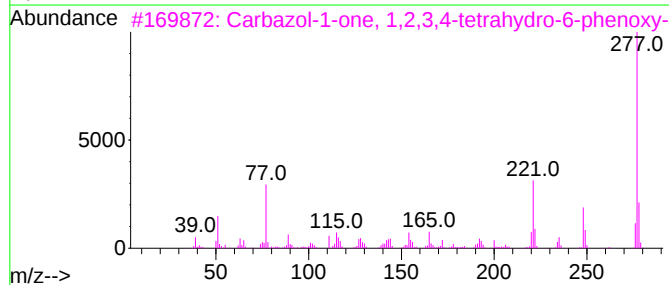
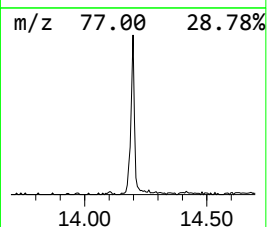
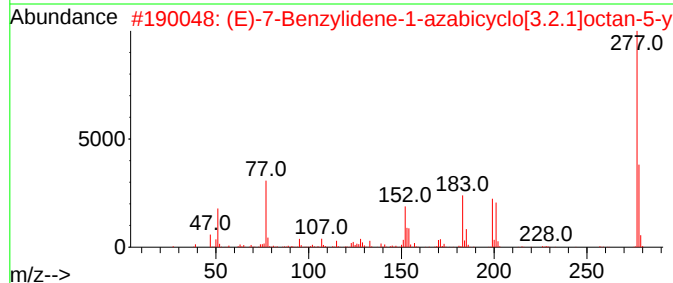
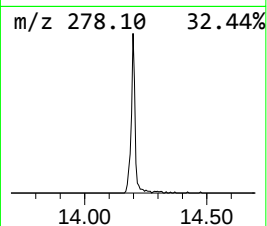
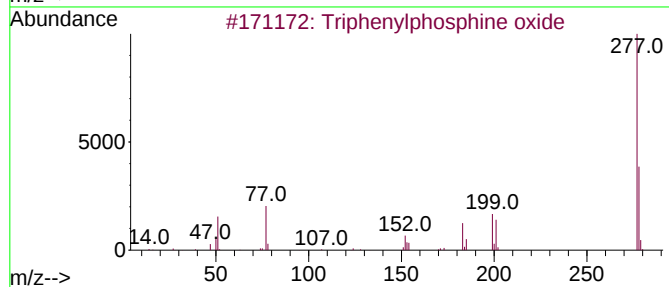
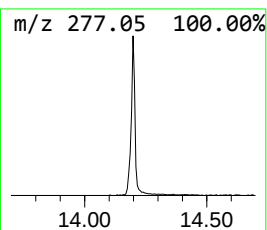
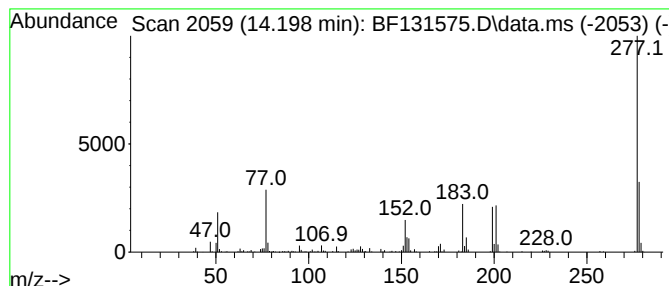
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	12.58 ng	298928	Chrysene-d12	14.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	90
3			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	35
5			cyclopenta[d][1,3]thiazine-2,4-d...	277	C13H11NS3	1000397-11-2	25



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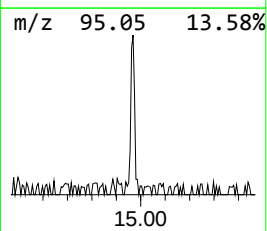
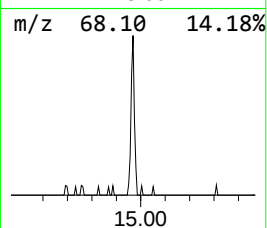
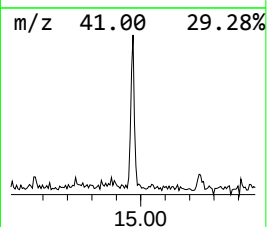
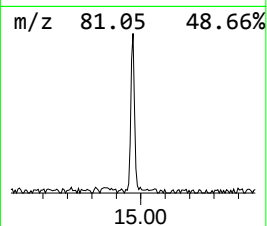
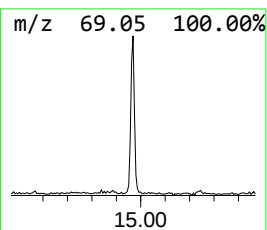
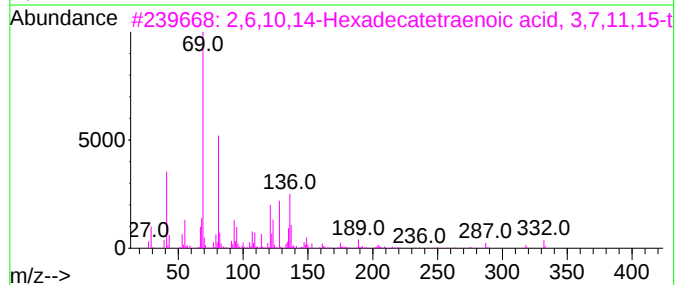
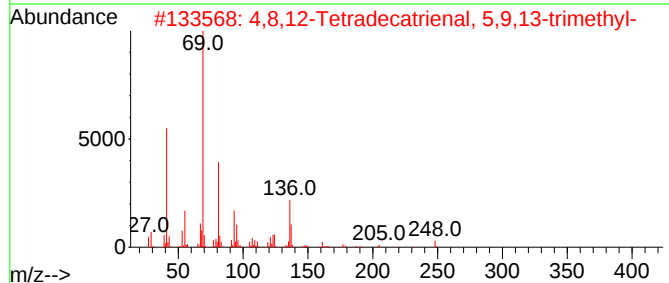
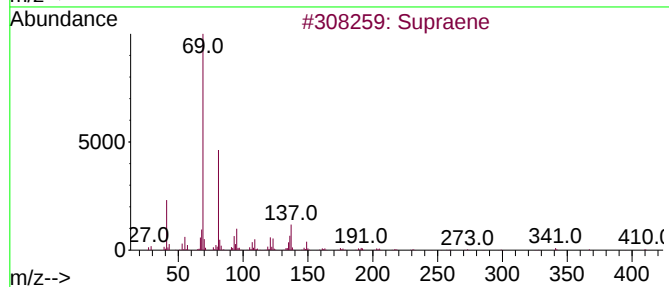
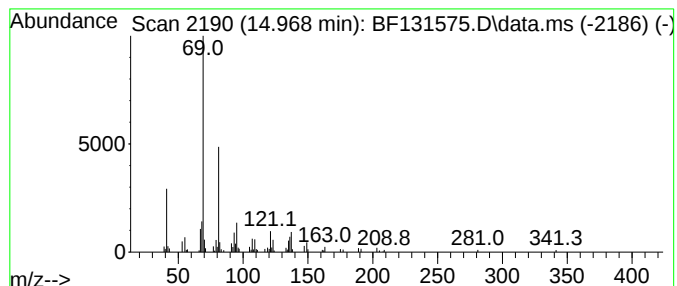
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	5.01 ng	88564	Perylene-d12	15.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	59
5			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120922\
Data File : BF131575.D
Acq On : 09 Dec 2022 19:45
Operator : CG\JU
Sample : N5963-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBR200014-RB21197

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.240	36.2	ng	734391	1	6.904	405561	20.0
2-Pentanone, 4-...	5.140	15.5	ng	314169	1	6.904	405561	20.0
Caryophyllene	9.610	2.5	ng	80439	3	9.957	654312	20.0
Cyclohexene, 3-...	10.475	3.6	ng	116995	3	9.957	654312	20.0
Triphenylphosph...	14.198	12.6	ng	298928	5	14.104	475233	20.0
Supraene	14.968	5.0	ng	88564	6	15.615	353641	20.0