

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
 Data File : BF131401.D
 Acq On : 25 Nov 2022 18:10
 Operator : CG\JU
 Sample : N5741-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-26

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131401.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	22	29	35	rVB	1671037	2138553	71.35%	11.159%
2	3.352	209	215	220	rBV	34634	63912	2.13%	0.333%
3	5.169	520	524	530	rVB	218300	237189	7.91%	1.238%
4	5.563	586	591	594	rBV	1351264	1302660	43.46%	6.797%
5	6.563	756	761	764	rBV	966095	828168	27.63%	4.321%
6	6.957	824	828	831	rVB	619646	553809	18.48%	2.890%
7	7.522	918	924	927	rBV	1742054	1723832	57.51%	8.995%
8	7.587	931	935	938	rVB	36569	34653	1.16%	0.181%
9	7.804	967	972	976	rVB2	72517	81290	2.71%	0.424%
10	8.245	1042	1047	1050	rBV	826940	702614	23.44%	3.666%
11	9.328	1225	1231	1234	rBV	3435950	2997471	100.00%	15.641%
12	9.433	1244	1249	1253	rVB2	58467	66776	2.23%	0.348%
13	9.892	1321	1327	1332	rBV	87489	90141	3.01%	0.470%
14	10.010	1343	1347	1350	rVB	986128	800992	26.72%	4.180%
15	10.198	1373	1379	1384	rBV3	31211	38407	1.28%	0.200%
16	10.728	1465	1469	1472	rVB	100830	83542	2.79%	0.436%
17	10.804	1477	1482	1485	rBV	2116085	1904927	63.55%	9.940%
18	11.504	1597	1601	1605	rBV	988093	804733	26.85%	4.199%
19	12.027	1686	1690	1694	rBV	254473	238186	7.95%	1.243%
20	12.816	1821	1824	1831	rBV	169907	154785	5.16%	0.808%
21	13.104	1868	1873	1876	rBV	3224079	2860879	95.44%	14.928%
22	14.027	2023	2030	2041	rBV4	52114	152210	5.08%	0.794%
23	14.163	2049	2053	2057	rVB	619319	522009	17.41%	2.724%
24	14.257	2065	2069	2075	rVB	89959	94535	3.15%	0.493%
25	15.698	2309	2314	2318	rBV	358197	466603	15.57%	2.435%
26	15.733	2318	2320	2328	rVB2	35053	46730	1.56%	0.244%
27	16.210	2396	2401	2406	rBV2	27857	44059	1.47%	0.230%
28	16.762	2490	2495	2501	rBV4	25188	47246	1.58%	0.247%
29	17.409	2600	2605	2613	rBV4	20459	39173	1.31%	0.204%
30	18.186	2731	2737	2744	rVB5	16826	44034	1.47%	0.230%

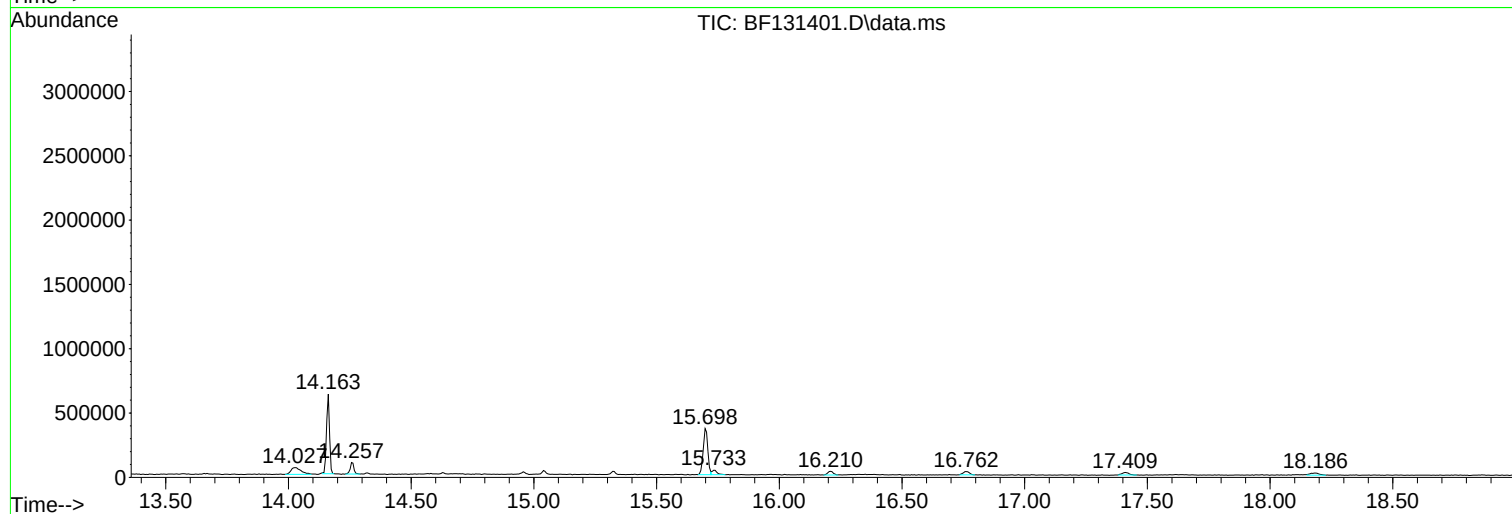
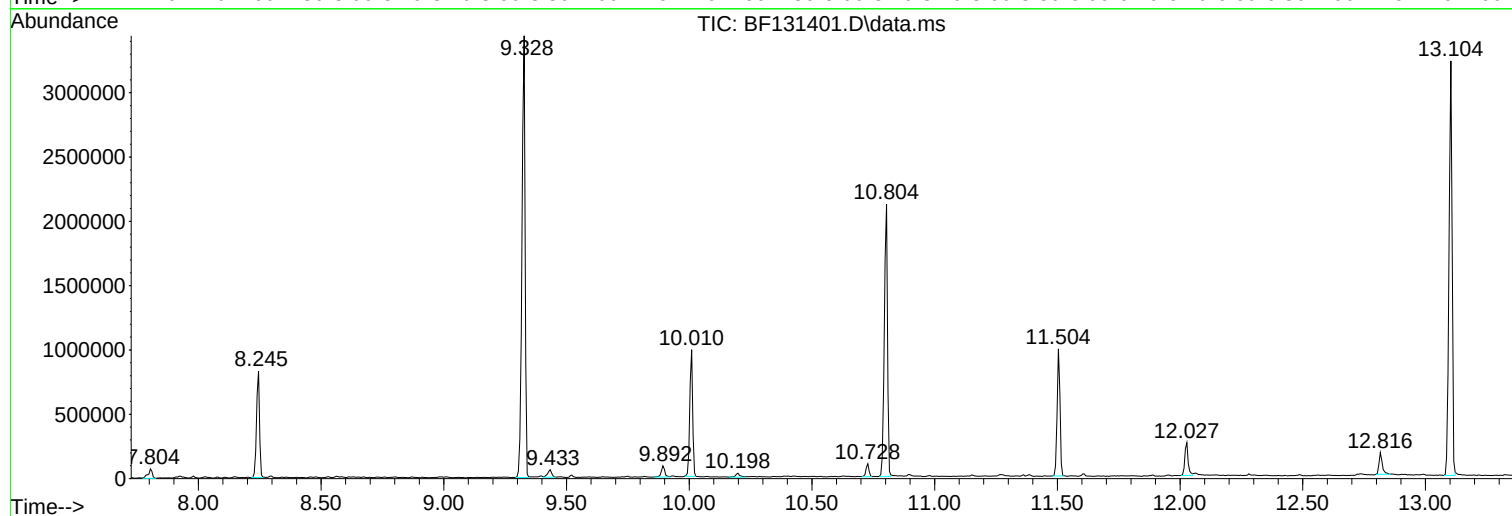
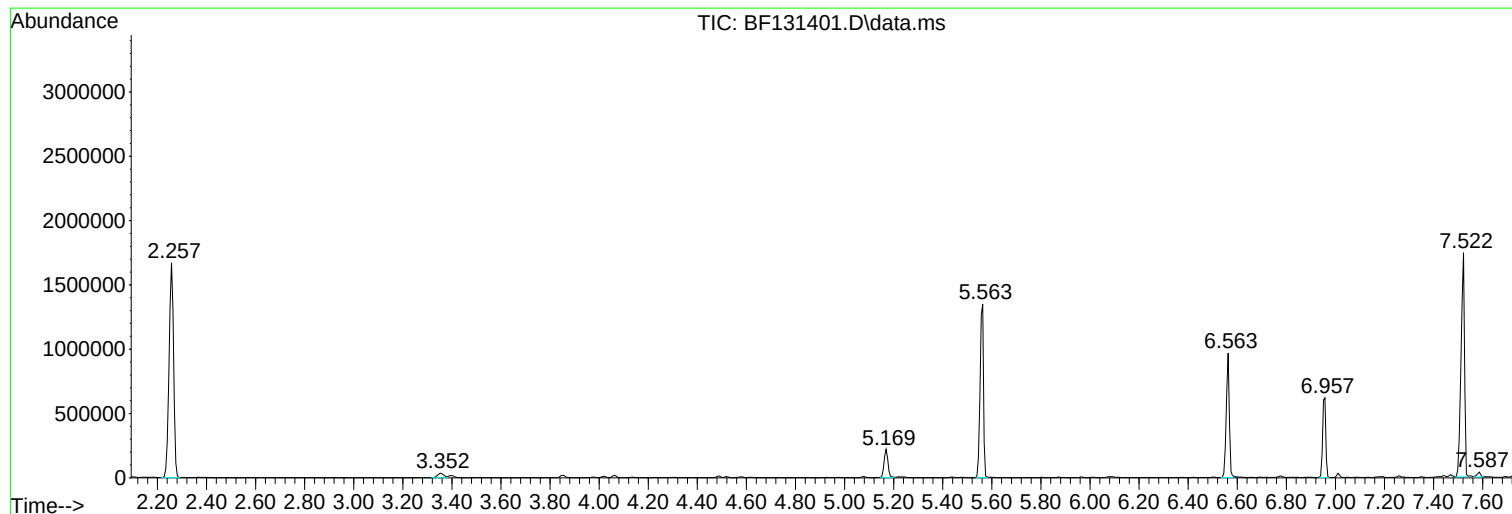
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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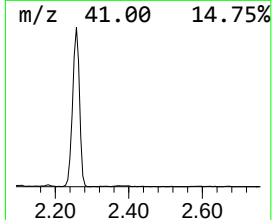
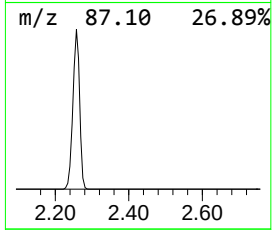
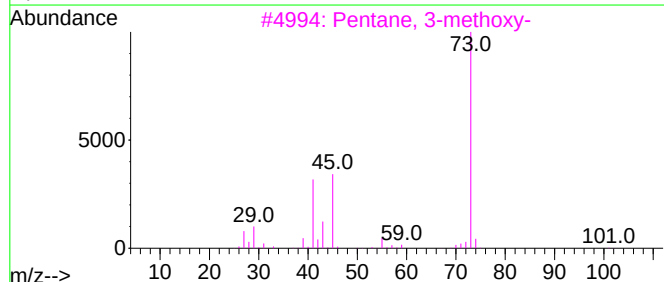
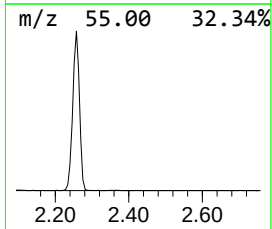
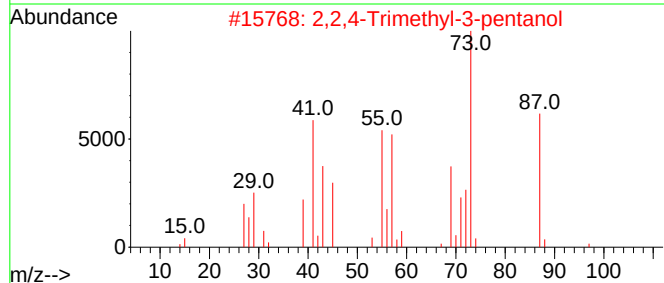
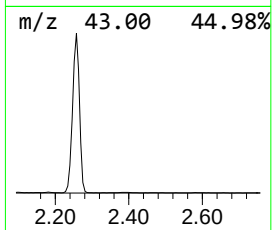
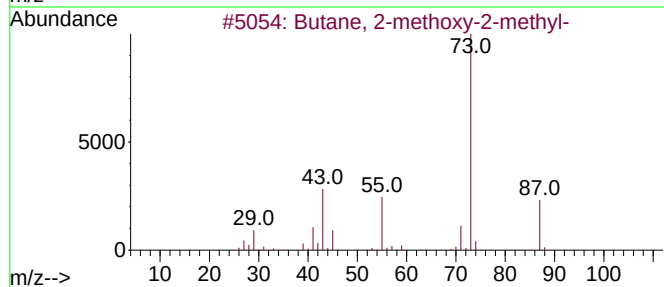
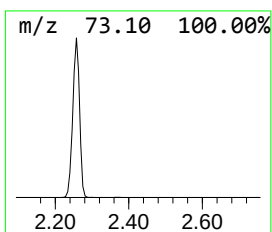
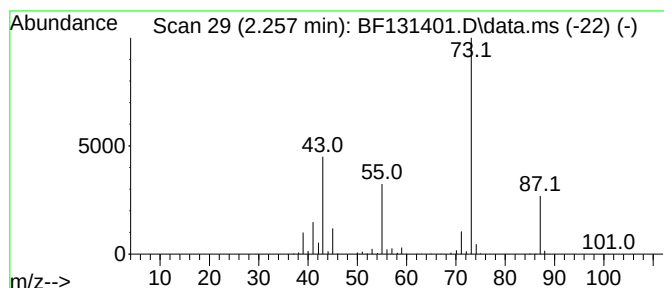
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.257	77.23 ng	2138550	1,4-Dichlorobenzene-d4	6.957

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	12
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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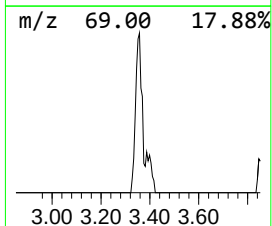
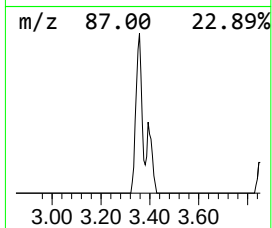
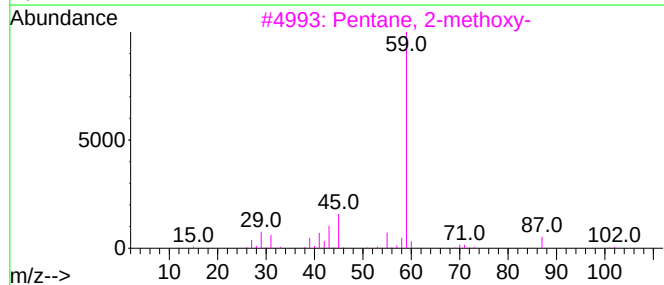
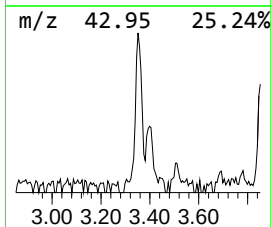
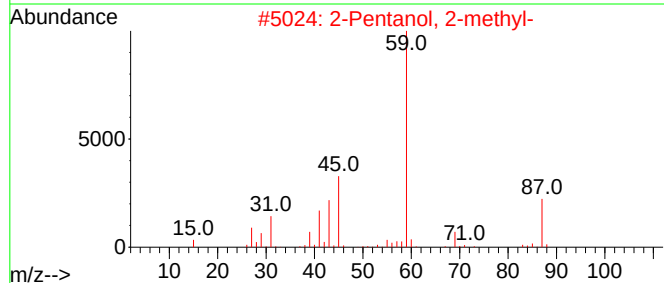
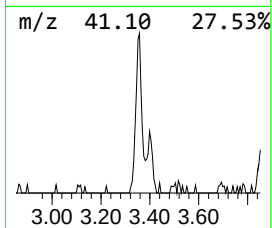
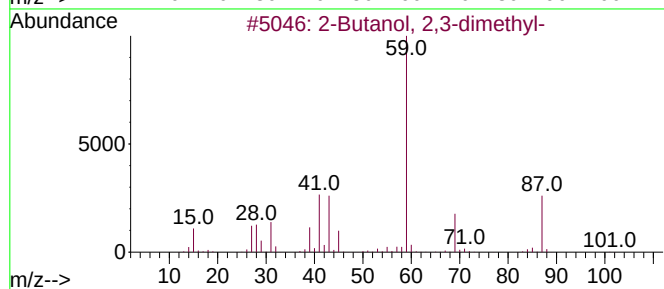
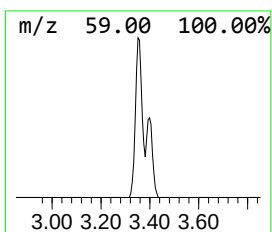
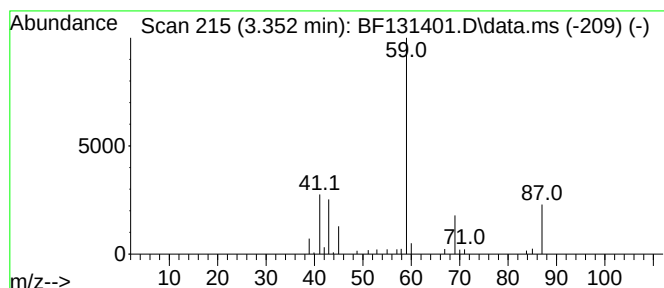
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Butanol, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.352	2.31 ng	63912	1,4-Dichlorobenzene-d4	6.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
3		Pentane, 2-methoxy-	102	C6H14O	006795-88-6	72
4		Amylene hydrate	88	C5H12O	000075-85-4	42
5		2-Decanol, methyl ether	172	C11H24O	1000333-83-9	36



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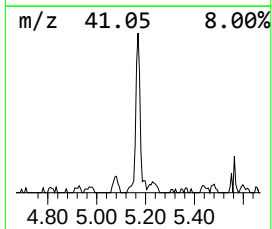
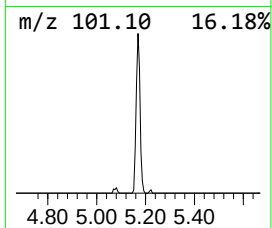
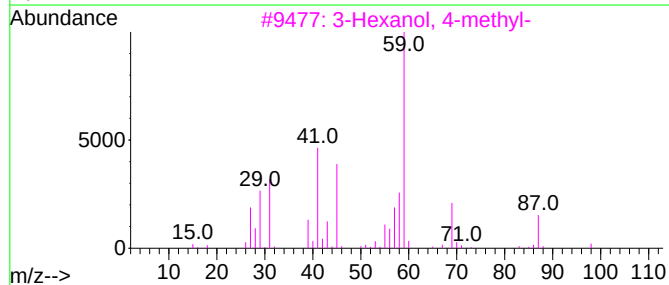
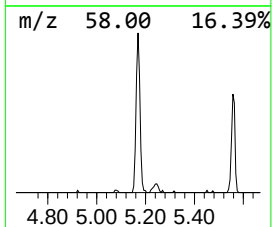
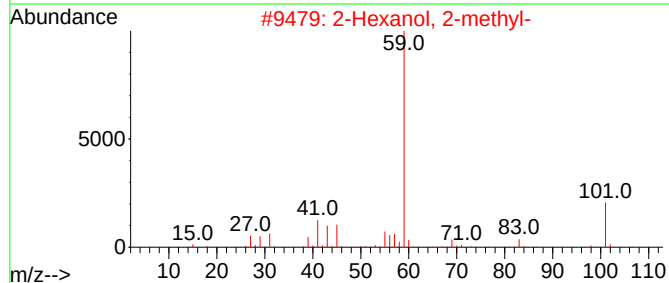
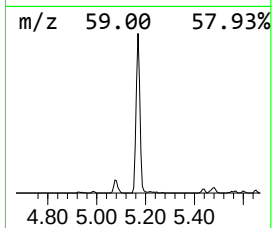
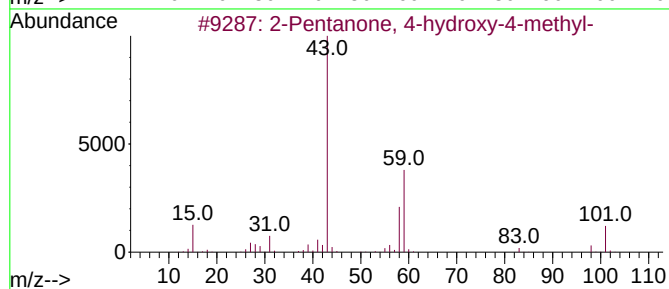
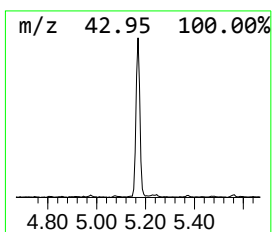
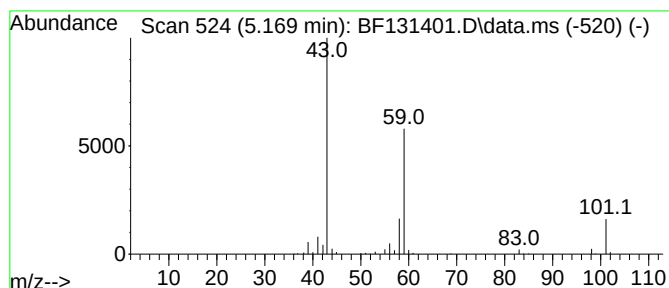
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.169	8.57 ng	237189	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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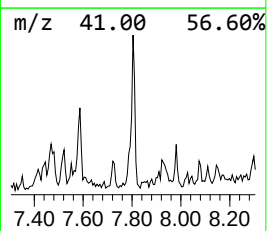
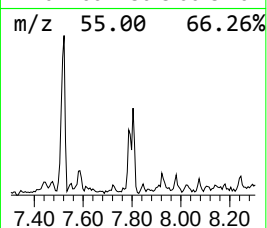
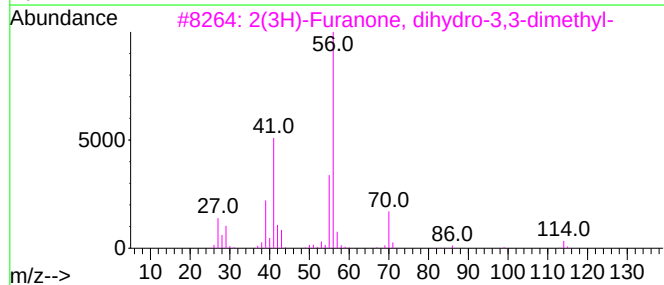
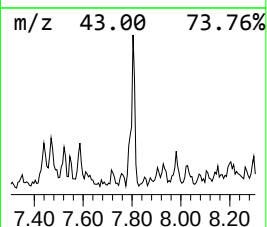
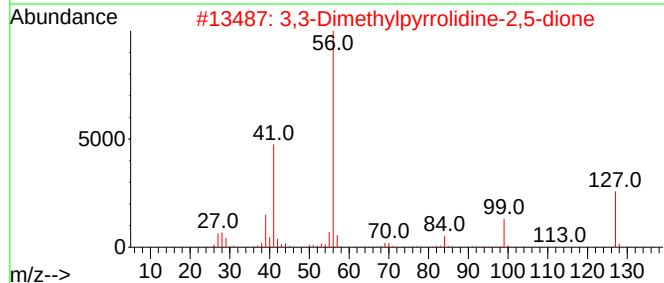
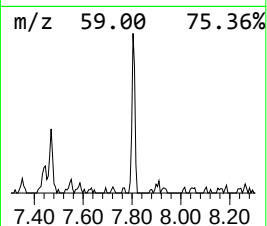
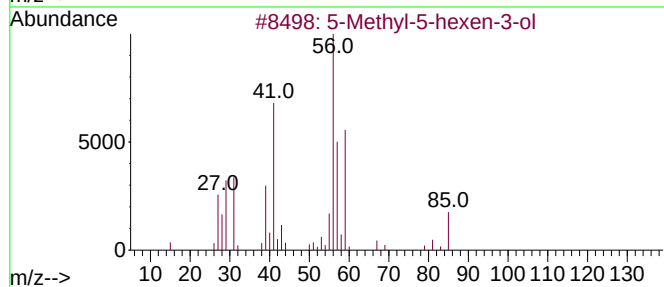
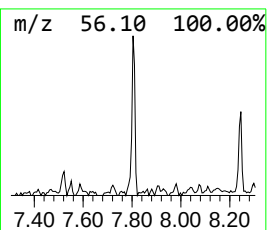
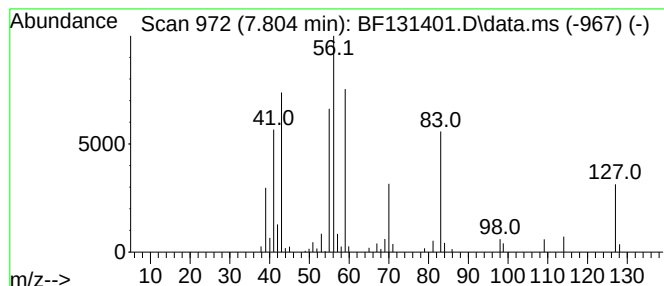
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown7.804 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.804	2.31 ng	81290	Naphthalene-d8	8.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	38
2			3,3-Dimethylpyrrolidine-2,5-dione	127	C6H9NO2	003437-29-4	27
3			2(3H)-Furanone, dihydro-3,3-dime...	114	C6H10O2	003709-08-8	25
4			2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	22
5			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	22



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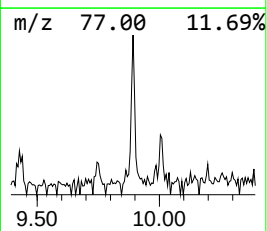
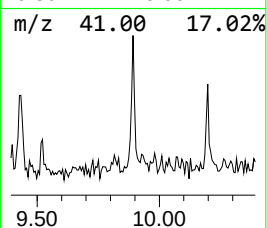
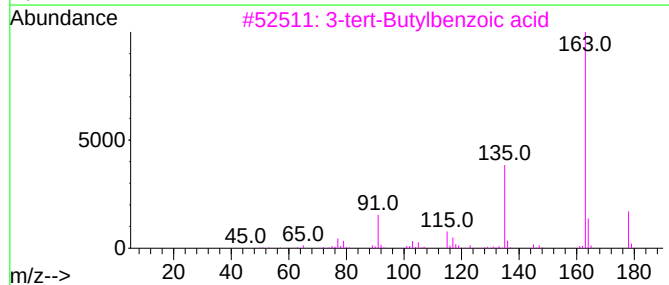
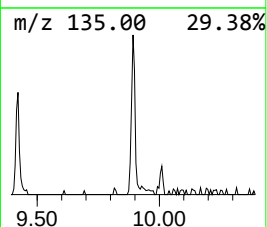
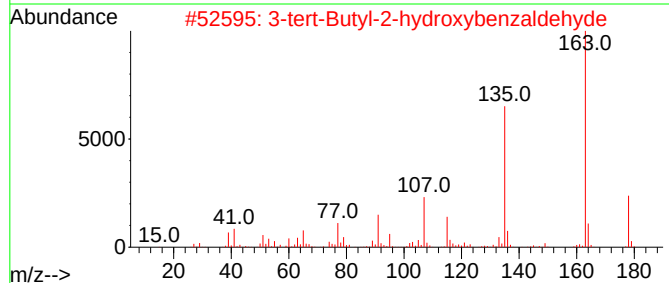
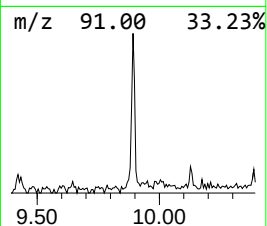
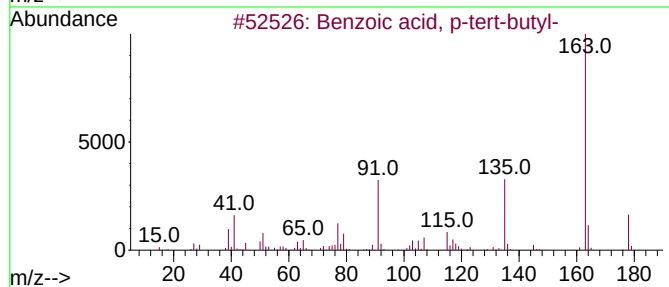
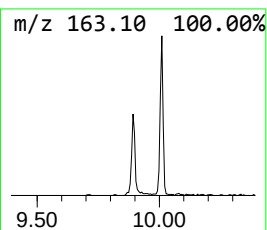
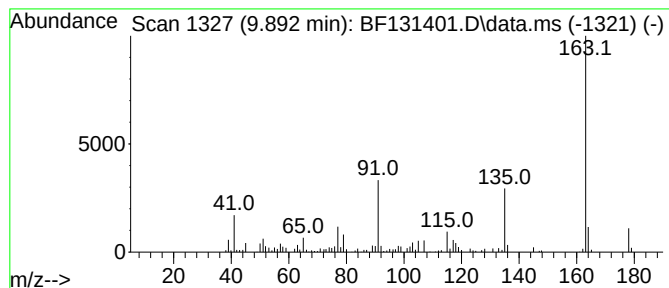
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzoic acid, p-tert-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.892	2.25 ng	90141	Acenaphthene-d10	10.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	95
2			3-tert-Butyl-2-hydroxybenzaldehyde	178	C11H14O2	024623-65-2	64
3			3-tert-Butylbenzoic acid	178	C11H14O2	007498-54-6	64
4			6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	64
5			Benzaldehyde, 5-(1,1-dimethyleth...	178	C11H14O2	002725-53-3	59



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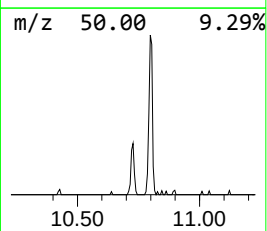
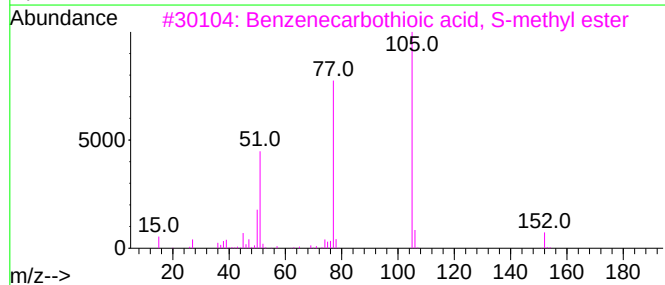
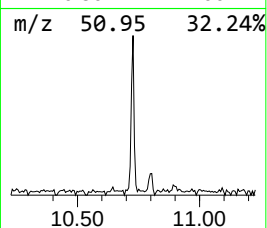
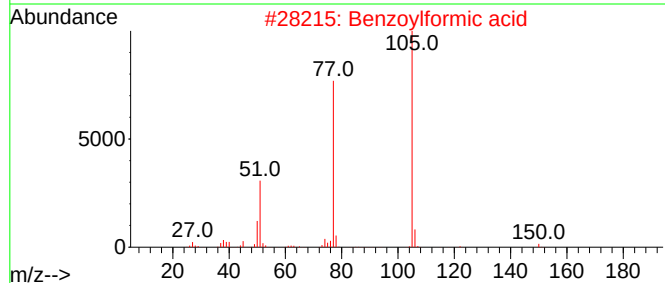
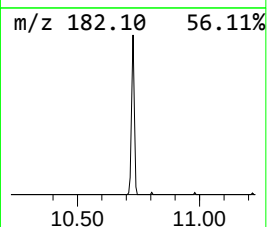
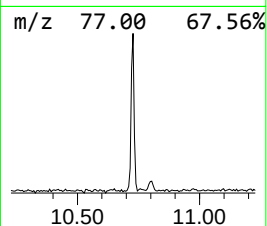
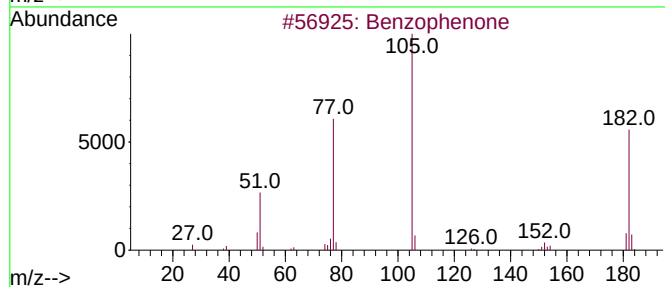
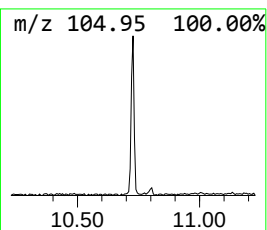
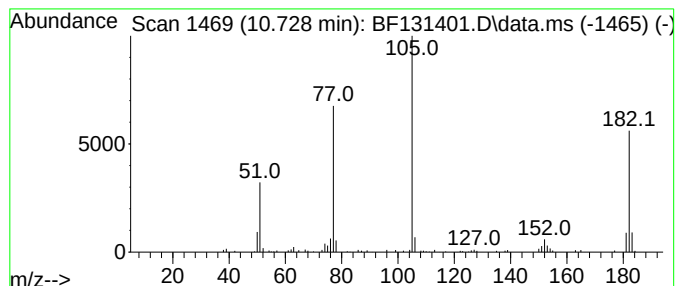
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.727	2.09 ng	83542	Acenaphthene-d10	10.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoylformic acid	150	C8H6O3	000611-73-4	53
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	47
5			2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131401.D
Acq On : 25 Nov 2022 18:10
Operator : CG\JU
Sample : N5741-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-26

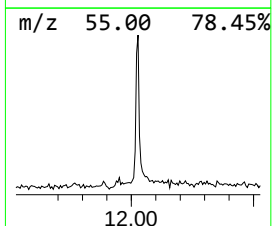
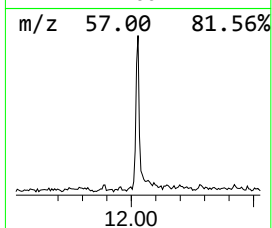
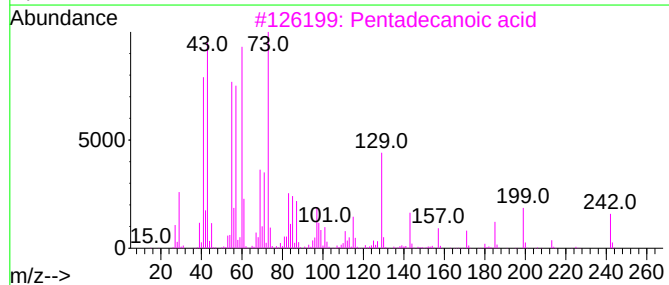
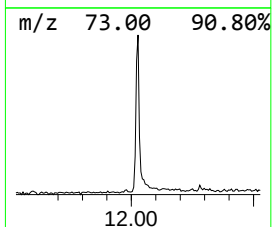
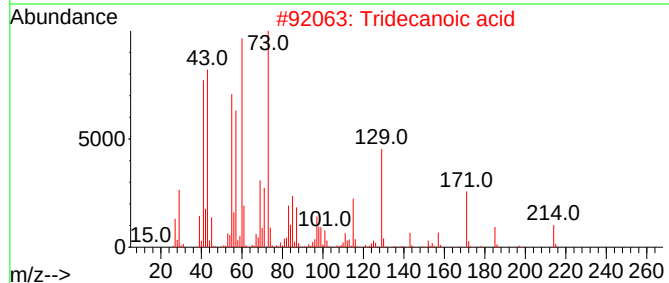
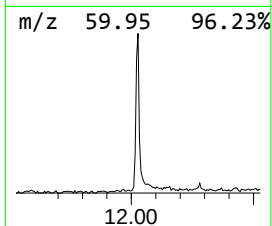
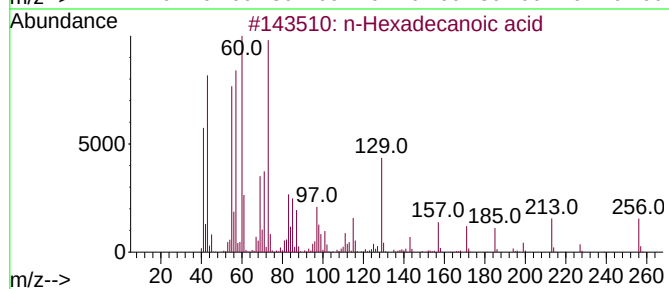
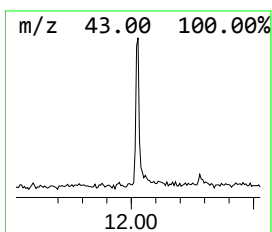
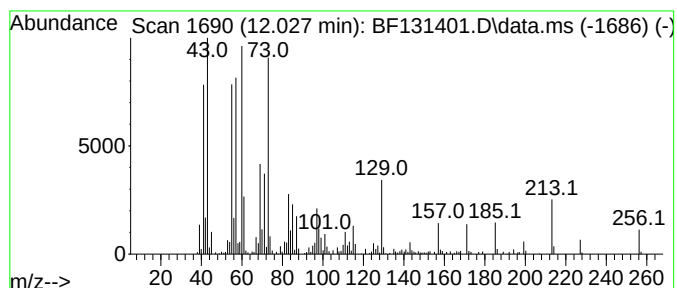
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.027	5.92 ng	238186	Phenanthrene-d10	11.504

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	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131401.D
Acq On : 25 Nov 2022 18:10
Operator : CG\JU
Sample : N5741-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

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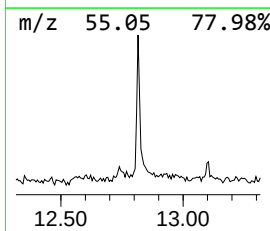
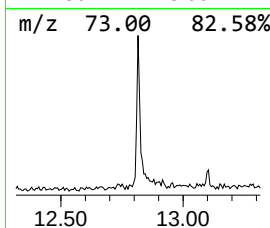
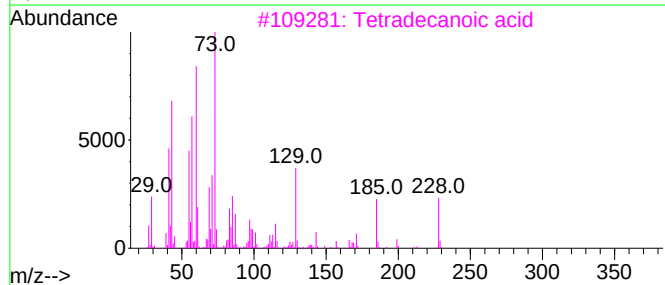
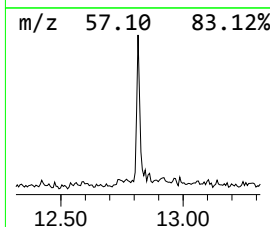
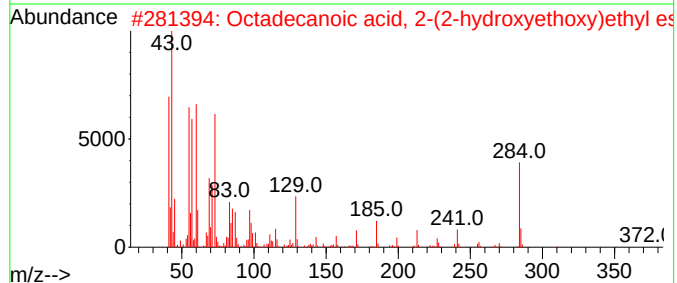
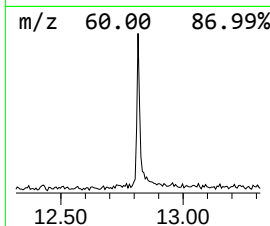
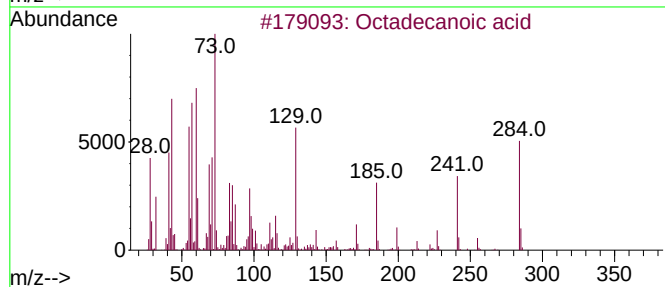
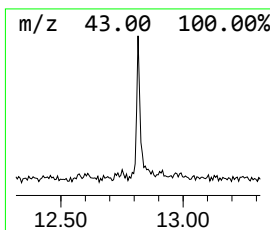
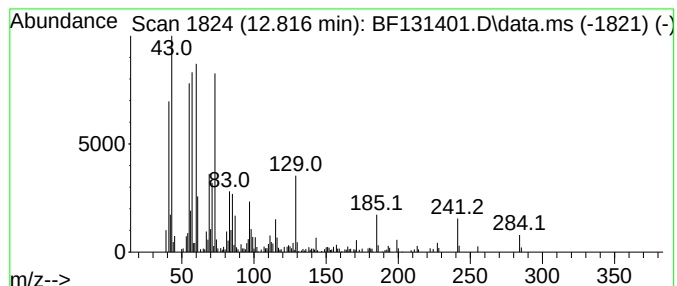
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.816	3.85 ng	154785	Phenanthrene-d10	11.504

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131401.D
Acq On : 25 Nov 2022 18:10
Operator : CG\JU
Sample : N5741-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

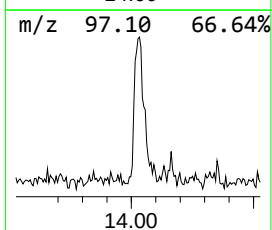
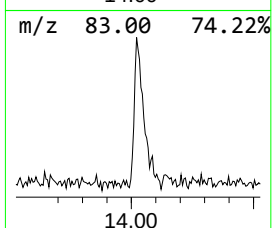
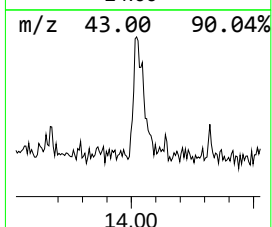
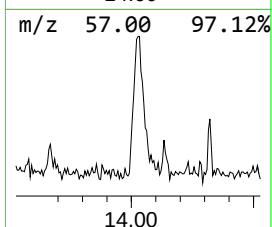
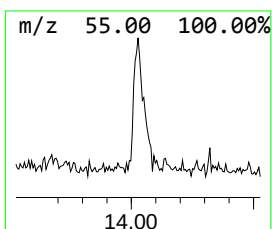
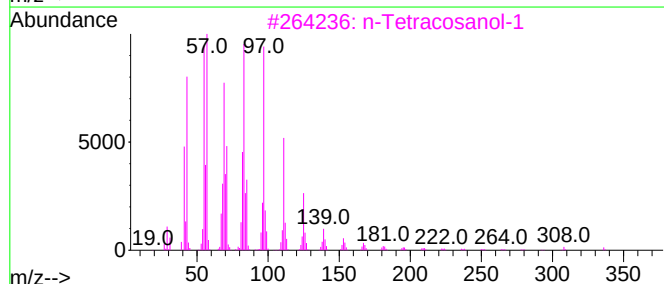
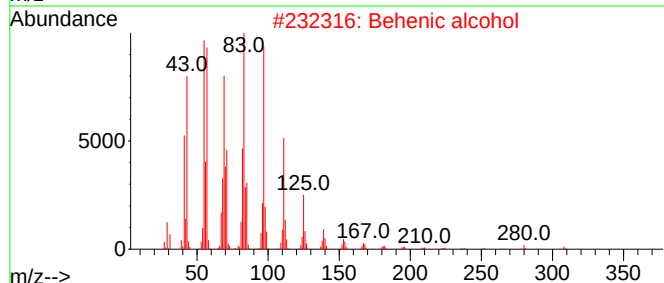
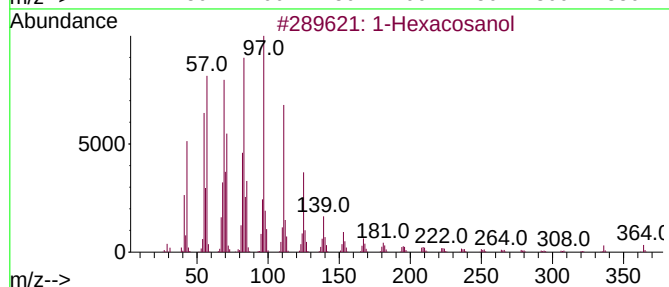
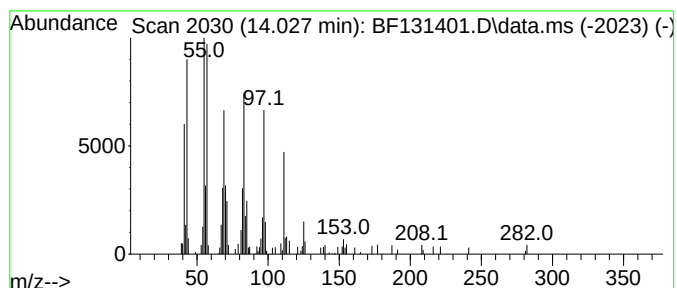
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.027	5.83 ng	152210	Chrysene-d12	14.163	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	87
2	Behenic alcohol	326	C22H46O	000661-19-8	83
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	83
4	1-Hexacosene	364	C26H52	018835-33-1	80
5	1-Heptacosanol	396	C27H56O	002004-39-9	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131401.D
Acq On : 25 Nov 2022 18:10
Operator : CG\JU
Sample : N5741-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-26

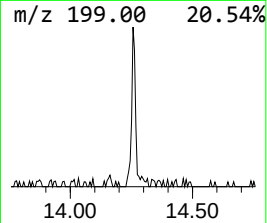
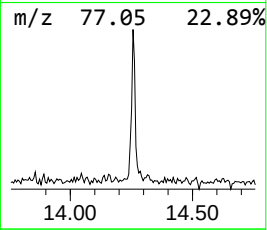
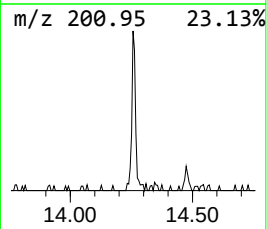
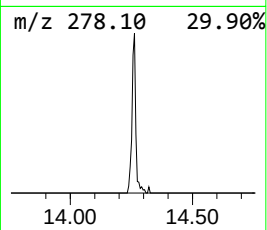
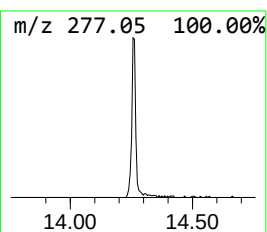
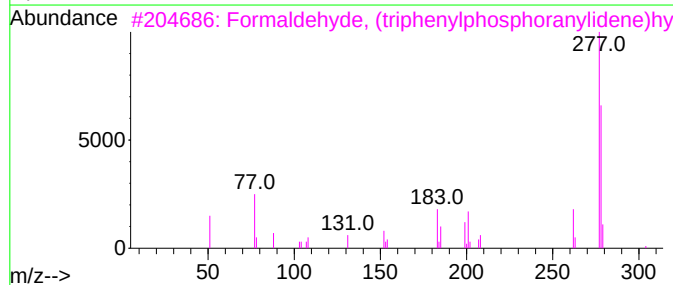
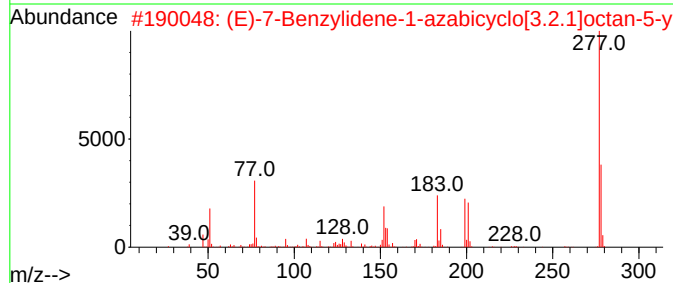
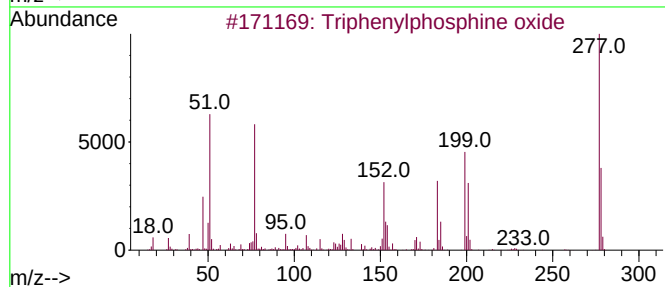
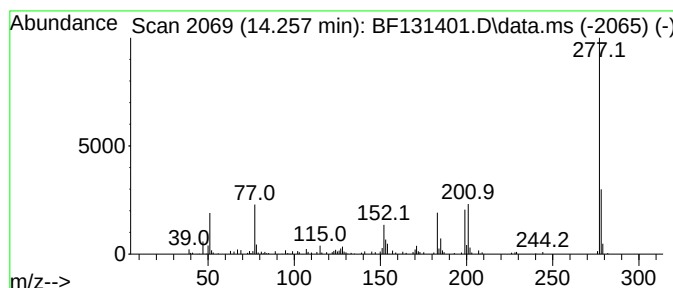
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	3.62 ng	94535	Chrysene-d12	14.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	78
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	38
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131401.D
Acq On : 25 Nov 2022 18:10
Operator : CG\JU
Sample : N5741-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-26

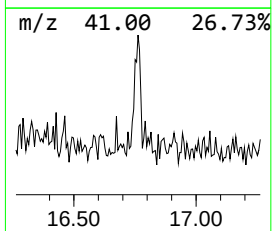
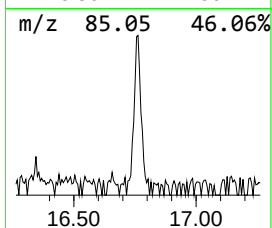
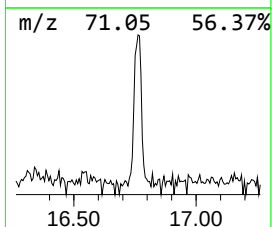
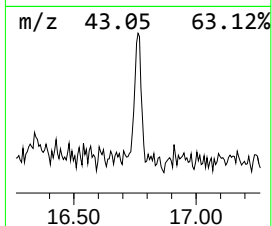
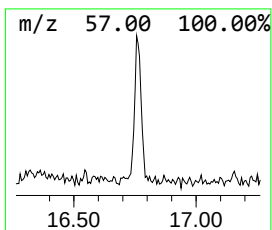
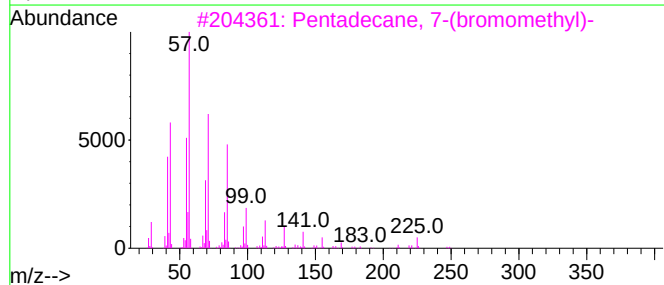
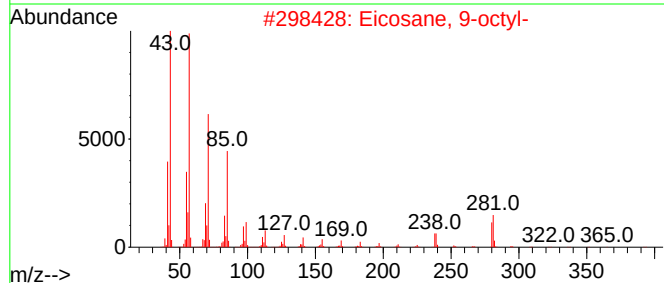
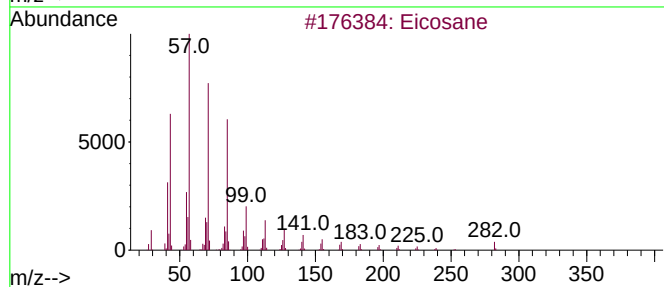
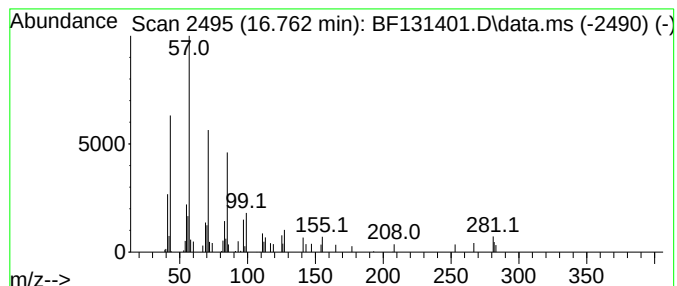
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	2.03 ng	47246	Perylene-d12	15.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Eicosane, 9-octyl-	394	C28H58	013475-77-9	86
3			Pentadecane, 7-(bromomethyl)-	304	C16H33Br	052997-43-0	80
4			5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	80
5			Hexatriacontane	507	C36H74	000630-06-8	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
Data File : BF131401.D
Acq On : 25 Nov 2022 18:10
Operator : CG\JU
Sample : N5741-08
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Butanol, 2,3-...	3.352	2.3	ng	63912	1	6.957	553809	20.0
2-Pentanone, 4-...	5.169	8.6	ng	237189	1	6.957	553809	20.0
unknown7.804	7.804	2.3	ng	81290	2	8.245	702614	20.0
Benzoic acid, p...	9.892	2.3	ng	90141	3	10.010	800992	20.0
Benzophenone	10.727	2.1	ng	83542	3	10.010	800992	20.0
n-Hexadecanoic ...	12.027	5.9	ng	238186	4	11.504	804733	20.0
Octadecanoic acid	12.816	3.9	ng	154785	4	11.504	804733	20.0
1-Hexacosanol	14.027	5.8	ng	152210	5	14.163	522009	20.0
Triphenylphosph...	14.257	3.6	ng	94535	5	14.163	522009	20.0
Eicosane	16.762	2.0	ng	47246	6	15.698	466603	20.0