

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
 Data File : BF126157.D
 Acq On : 12 Nov 2021 15:23
 Operator : JU/CG
 Sample : M4572-06
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 6

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-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.051	498	504	507	rBV	1900451	2271855	31.44%	6.401%
2	5.181	522	526	531	rBV	75971	105787	1.46%	0.298%
3	5.404	561	564	569	rBV2	112641	155482	2.15%	0.438%
4	5.457	569	573	576	rVV	2317232	1962982	27.17%	5.530%
5	6.087	676	680	684	rBV	406165	382421	5.29%	1.077%
6	6.463	740	744	753	rBV	1236724	999845	13.84%	2.817%
7	6.839	805	808	812	rBV	1045906	789544	10.93%	2.224%
8	6.904	816	819	830	rBV	268454	295908	4.10%	0.834%
9	7.404	896	904	907	rBV	3146827	3115694	43.12%	8.778%
10	7.592	932	936	942	rBV3	68811	85825	1.19%	0.242%
11	7.722	954	958	966	rBV	818476	767930	10.63%	2.164%
12	7.839	974	978	986	rBV	203150	198957	2.75%	0.561%
13	8.033	1007	1011	1023	rBV2	83842	131621	1.82%	0.371%
14	8.128	1023	1027	1030	rBV	1118747	1018785	14.10%	2.870%
15	8.351	1062	1065	1072	rVB	404898	337409	4.67%	0.951%
16	8.910	1157	1160	1170	rVB	67700	98445	1.36%	0.277%
17	9.204	1205	1210	1213	rBV	7231676	5784209	80.05%	16.296%
18	9.880	1321	1325	1328	rBV	1516511	1257243	17.40%	3.542%
19	9.974	1338	1341	1355	rBV	200019	240515	3.33%	0.678%
20	10.669	1454	1459	1462	rBV	4708579	4087139	56.57%	11.515%
21	11.233	1552	1555	1558	rBV	170133	137808	1.91%	0.388%
22	11.363	1574	1577	1581	rBV	1599296	1381597	19.12%	3.892%
23	11.727	1635	1639	1642	rBV	260390	204117	2.82%	0.575%
24	11.904	1665	1669	1680	rBV	392193	405188	5.61%	1.142%
25	12.957	1843	1848	1851	rBV	8380433	7225458	100.00%	20.356%
26	13.886	2002	2006	2016	rVB4	44515	86967	1.20%	0.245%
27	14.004	2022	2026	2030	rVB	1371316	1174999	16.26%	3.310%
28	15.468	2270	2275	2279	rBV	687791	790980	10.95%	2.228%

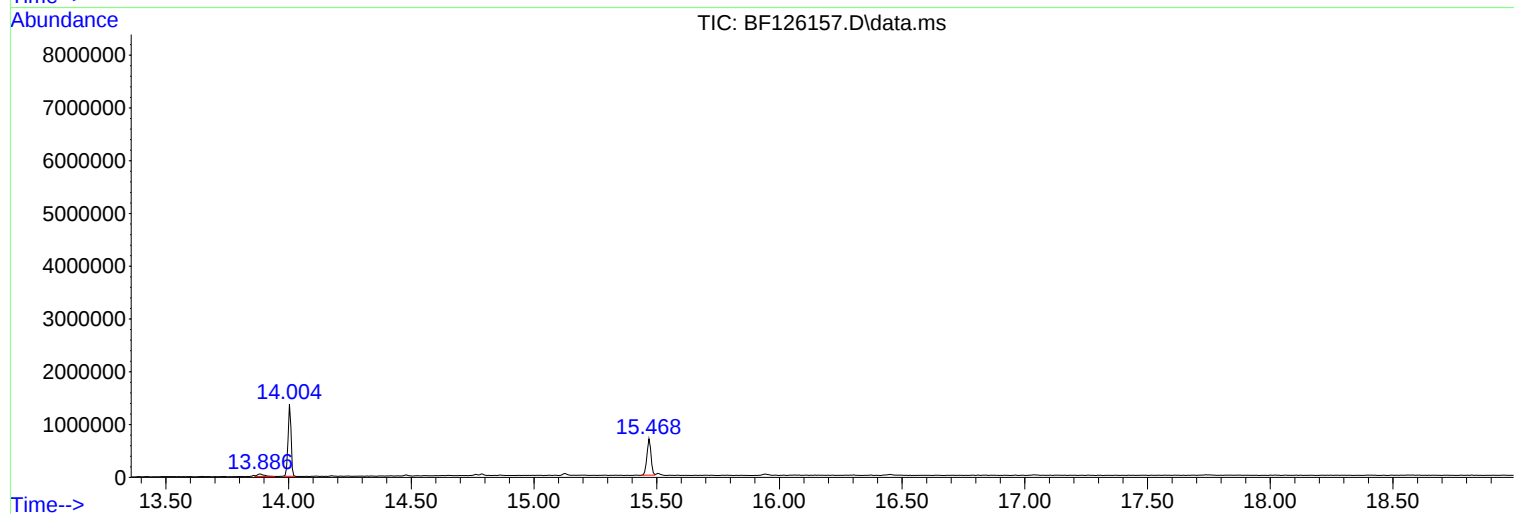
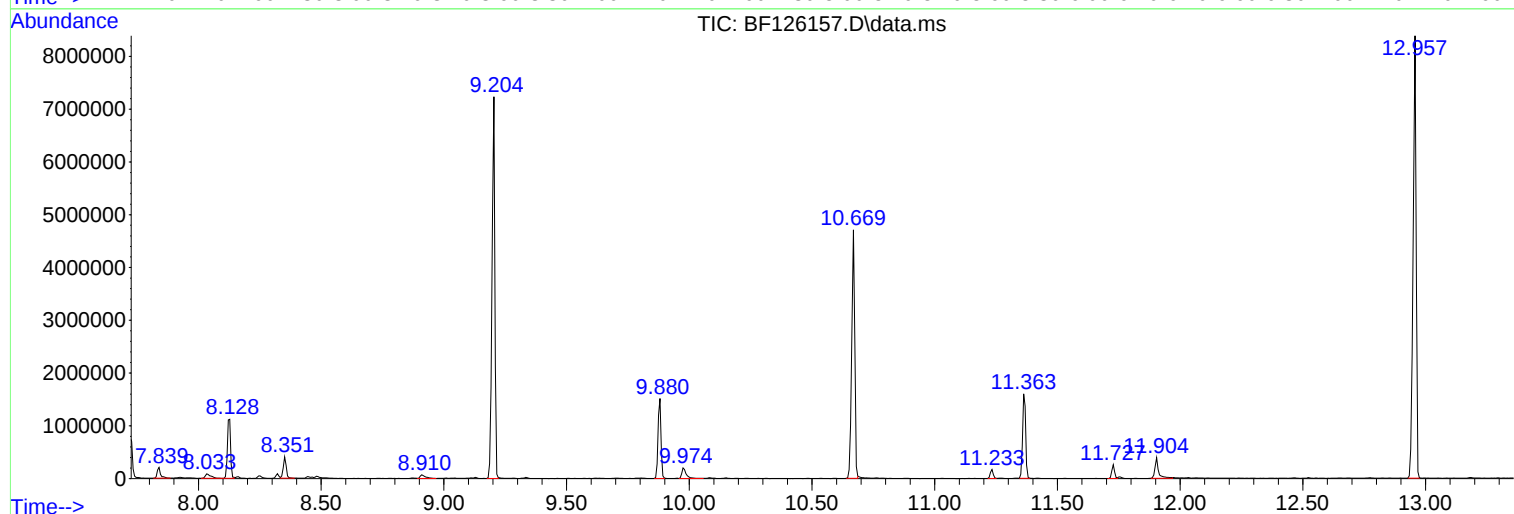
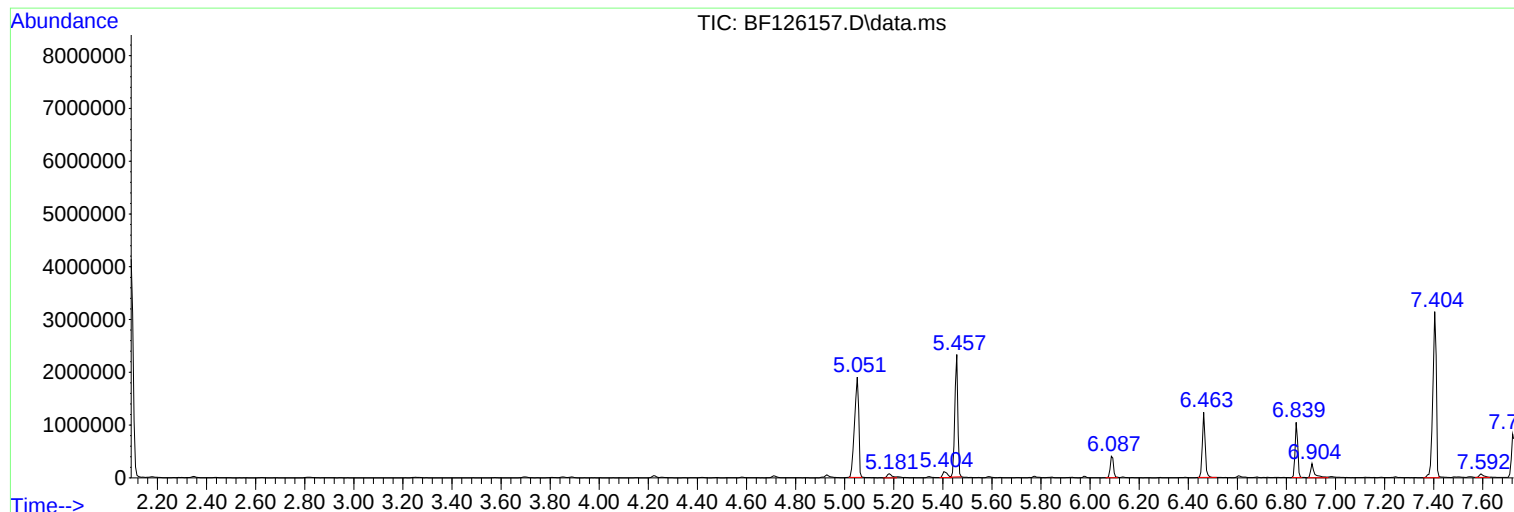
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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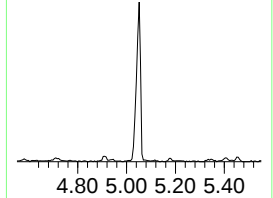
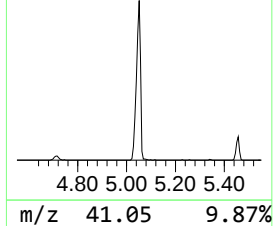
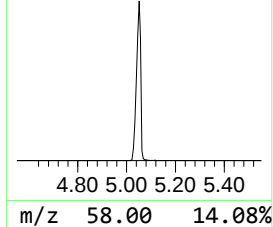
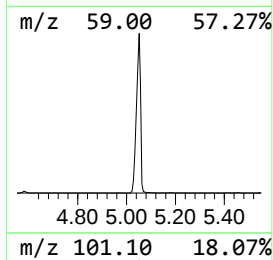
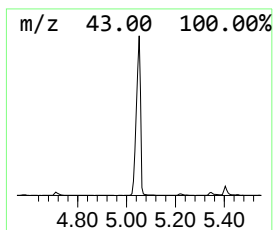
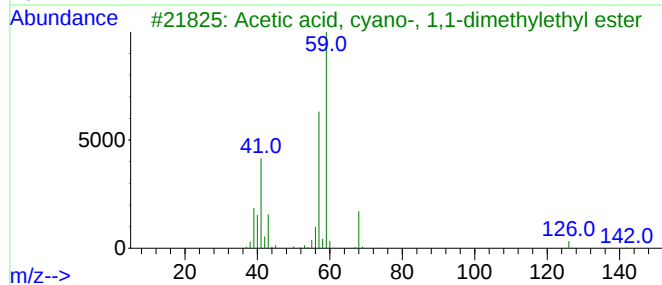
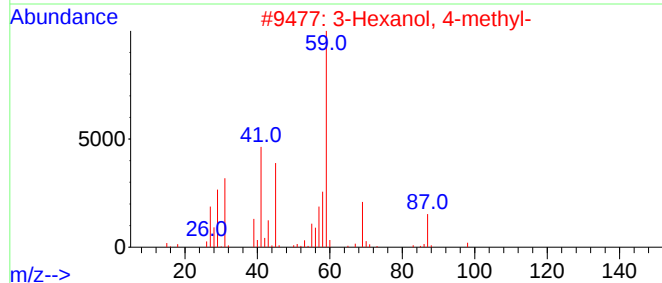
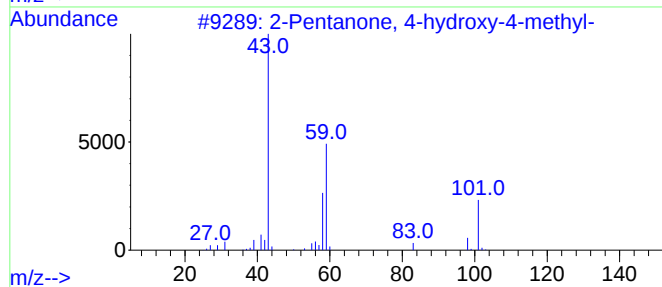
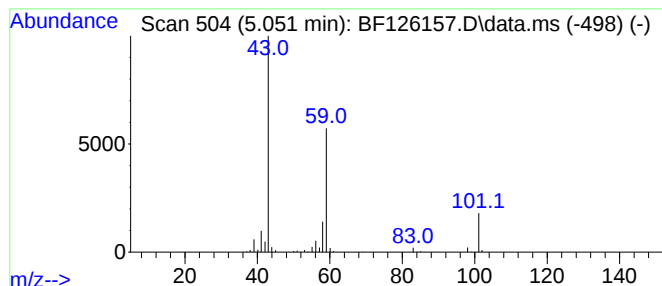
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.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.
5.051	57.55 ng	2271860	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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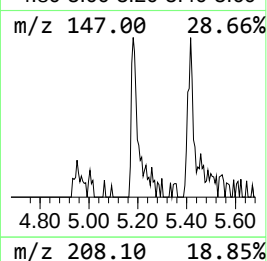
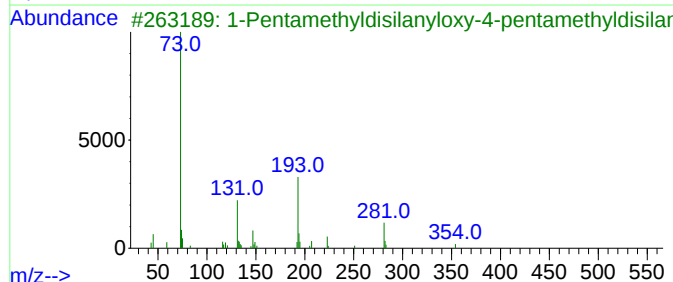
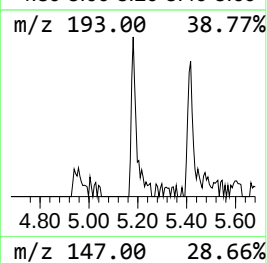
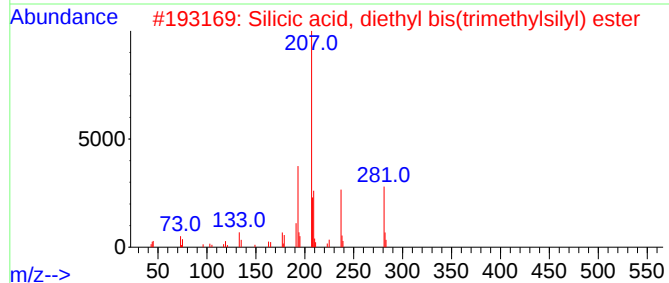
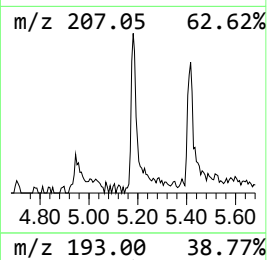
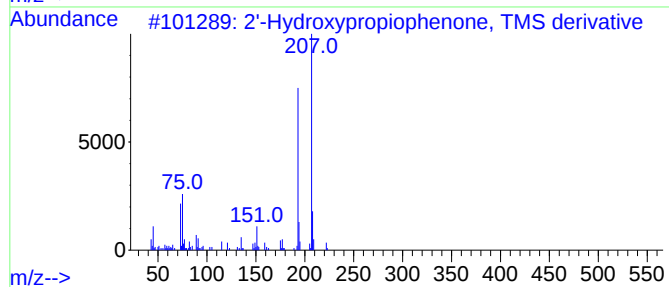
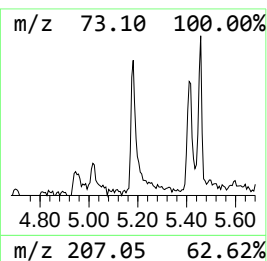
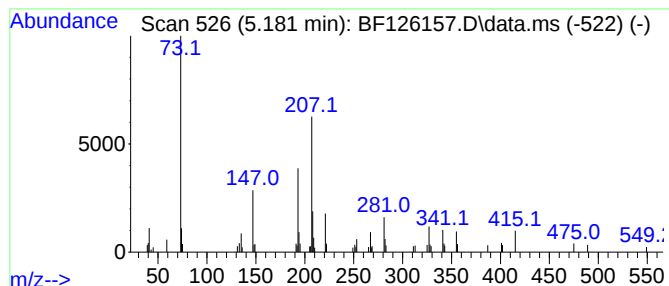
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Peak Number 2 unknown-5.181 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	2.68 ng	105787	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2'-Hydroxypropiophenone, TMS der...	222	C12H18O2Si	033342-87-9	43		
2	Silicic acid, diethyl bis(trimet...	296	C10H28O4Si3	003555-45-1	37		
3	1-Pentamethyldisilanyloxy-4-pent...	354	C16H34OSi4	1000427-15-7	22		
4	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	22		
5	5,5'-Di(ethoxycarbonyl)-3,3'-dim...	402	C23H34N2O4	102586-97-0	16		



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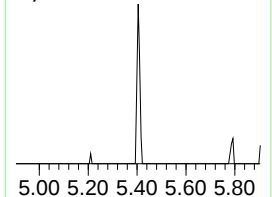
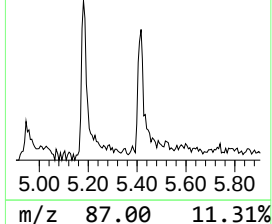
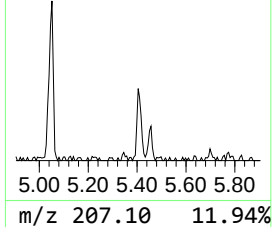
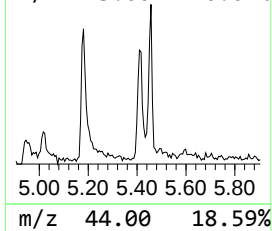
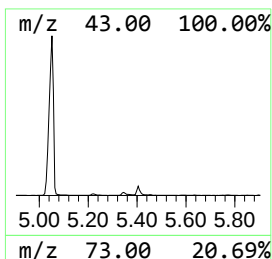
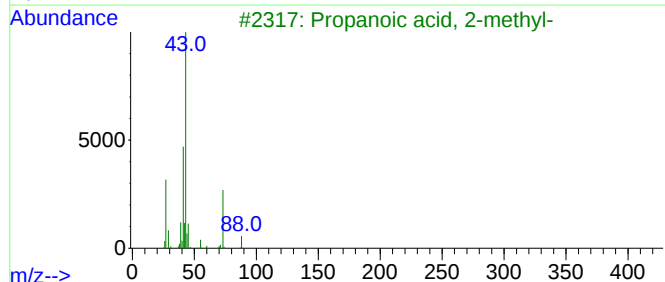
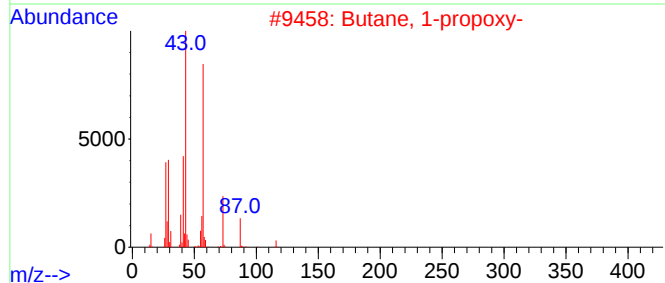
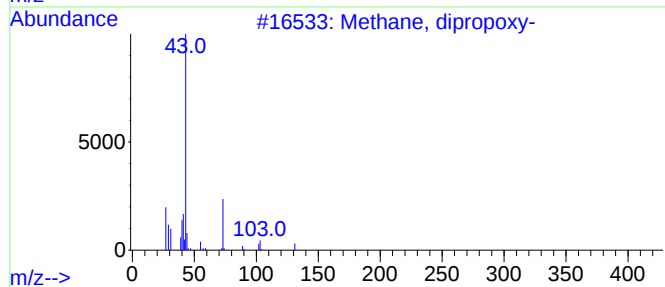
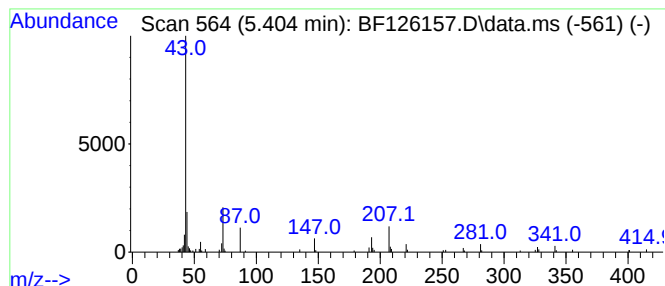
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Peak Number 3 unknown5.404 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.404	3.94 ng	155482	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, dipropoxy-	132	C7H16O2	000505-84-0	9
2			Butane, 1-propoxy-	116	C7H16O	003073-92-5	9
3			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9
4			Di-n-propyl ether	102	C6H14O	000111-43-3	9
5			4-Amino-furazan-3-carboxylic aci...	213	C7H11N5O3	347355-79-7	9



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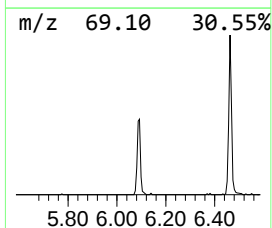
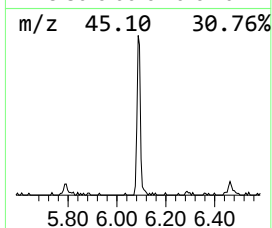
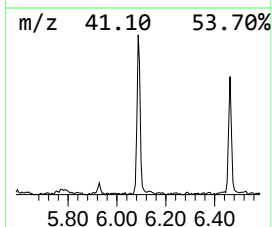
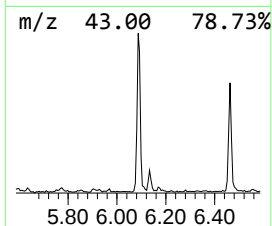
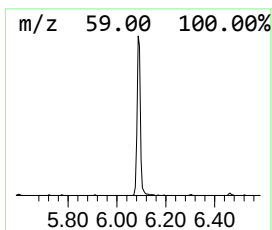
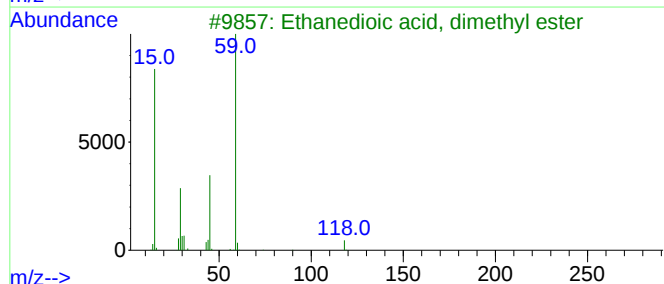
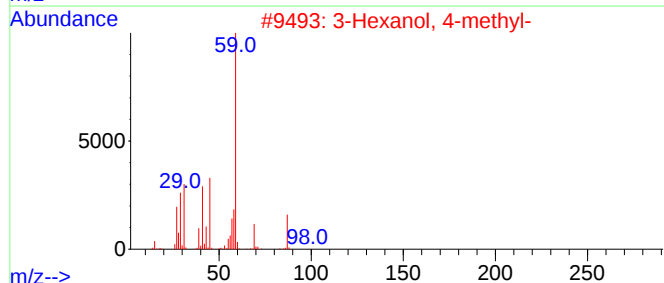
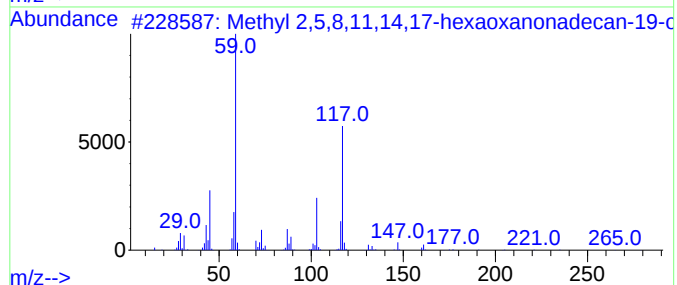
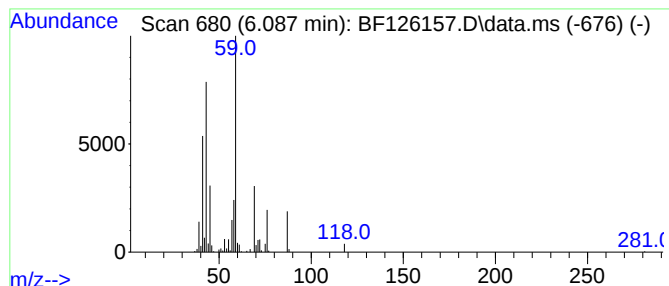
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Peak Number 4 Methyl 2,5,8,11,14,17-hexao... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.087	9.69 ng	382421	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 2,5,8,11,14,17-hexaoxonon...	324	C14H28O8	1000366-81-4	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	50
3			Ethanedioic acid, dimethyl ester	118	C4H6O4	000553-90-2	49
4			3-Pentanol	88	C5H12O	000584-02-1	47
5			Methyl 2,5,8,11,14,17,20-heptaox...	368	C16H32O9	1010366-81-3	42



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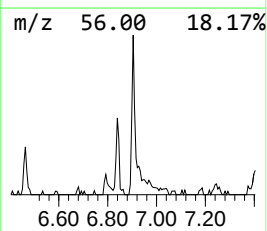
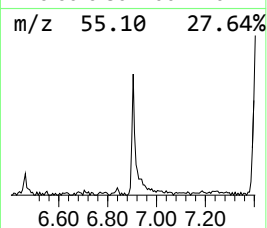
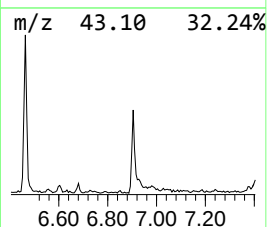
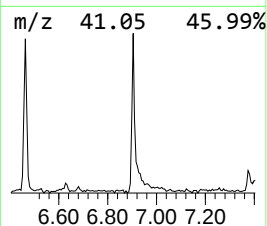
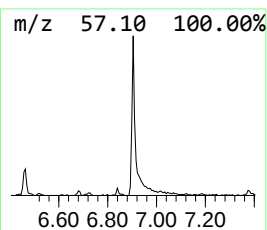
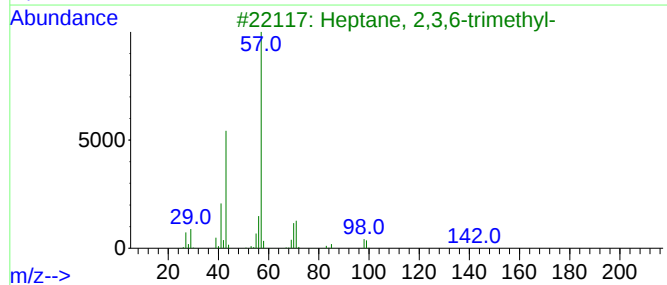
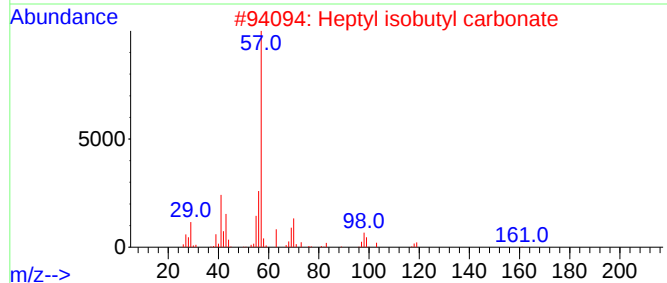
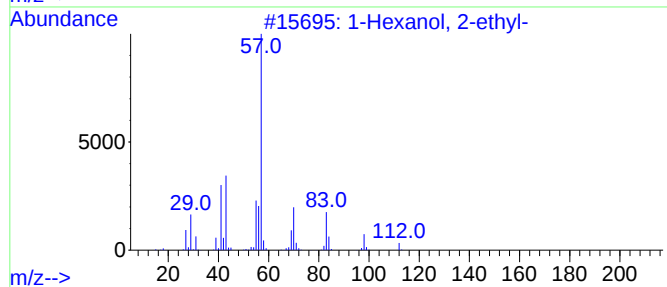
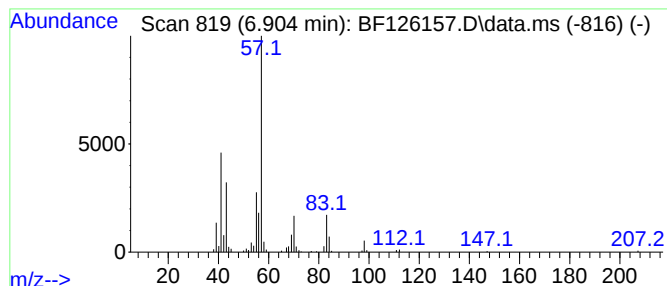
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.904	7.50 ng	295908	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	59
3			Heptane, 2,3,6-trimethyl-	142	C10H22	004032-93-3	59
4			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	47
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45



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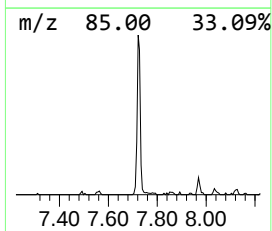
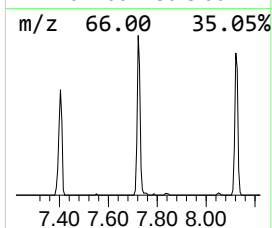
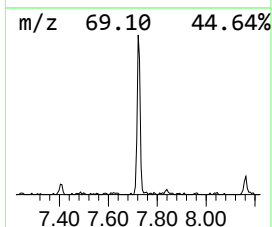
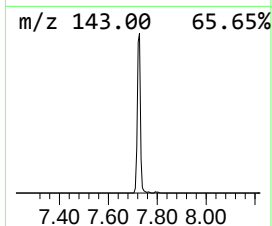
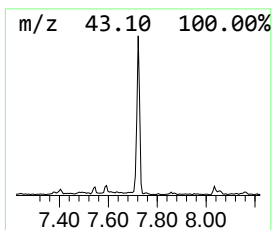
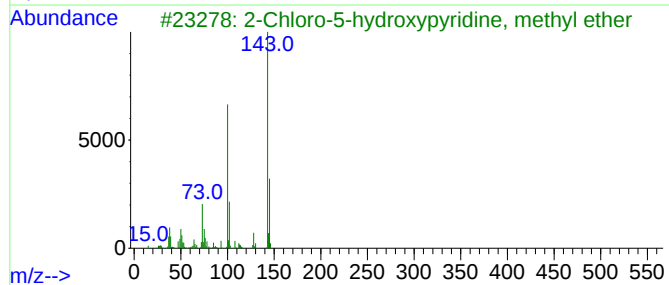
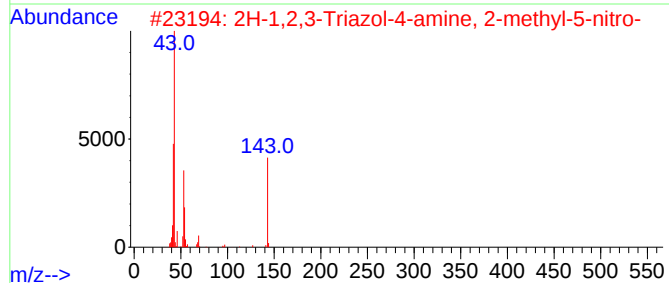
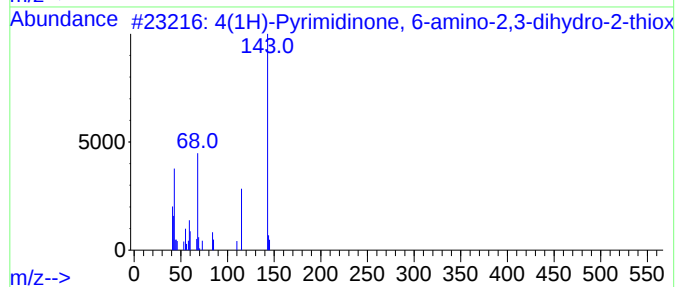
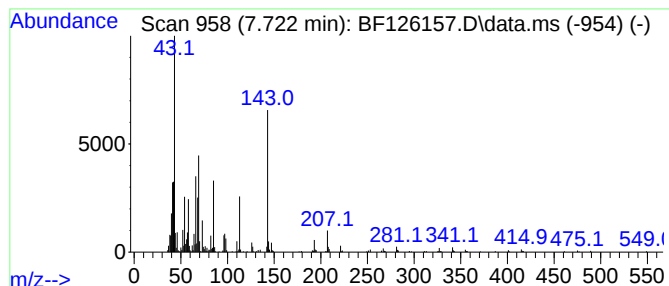
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.722 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.722	15.08 ng	767930	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	22		
2	2H-1,2,3-Triazol-4-amine, 2-meth...	143	C3H5N5O2	1000258-90-5	11		
3	2-Chloro-5-hydroxypyridine, meth...	143	C6H6ClNO	139585-48-1	10		
4	S-carbethoxymethyl-L-cysteine, N...	262	C10H18N2O4S	1000376-18-7	9		
5	Succinic acid, di(3,4-difluorobe...	370	C18H14F4O4	1000381-75-5	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
Data File : BF126157.D
Acq On : 12 Nov 2021 15:23
Operator : JU/CG
Sample : M4572-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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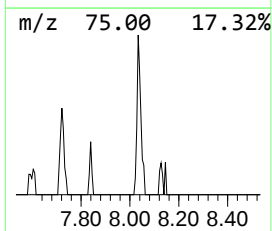
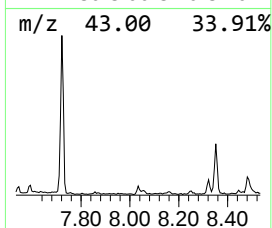
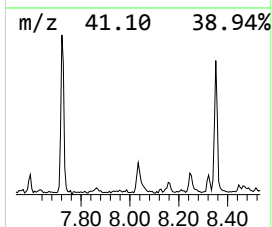
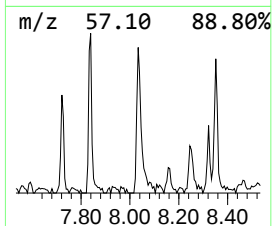
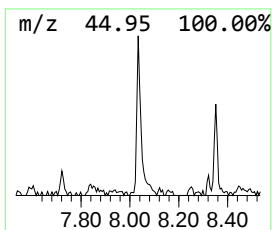
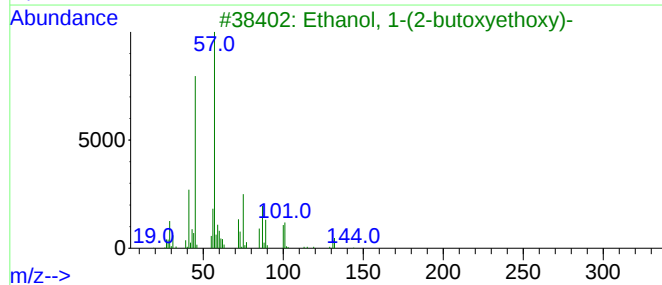
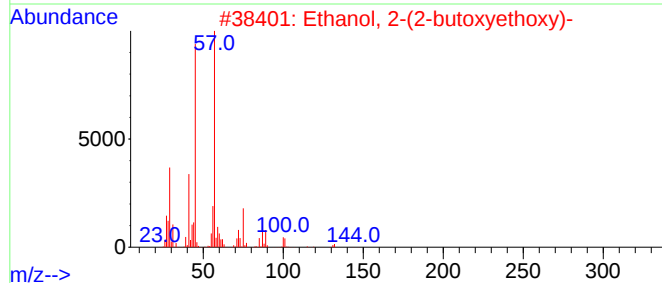
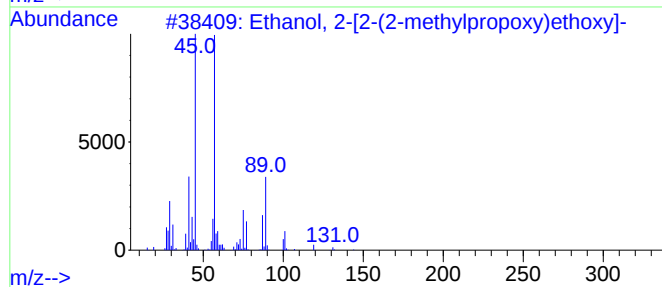
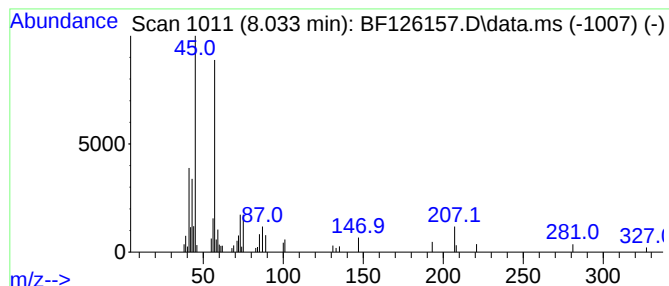
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ethanol, 2-[2-(2-methylprop... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.033	2.58 ng	131621	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
3			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	64
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
5			Triethylene glycol, TBDMS deriva...	264	C12H28O4Si	1000352-10-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
Data File : BF126157.D
Acq On : 12 Nov 2021 15:23
Operator : JU/CG
Sample : M4572-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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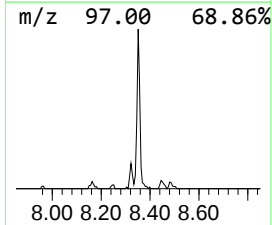
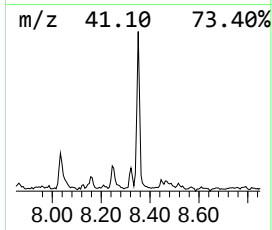
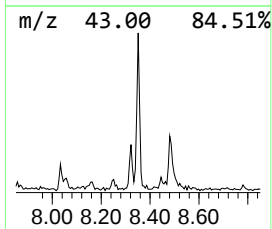
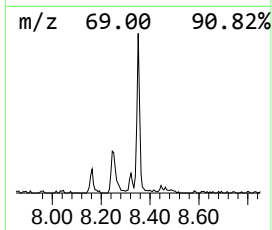
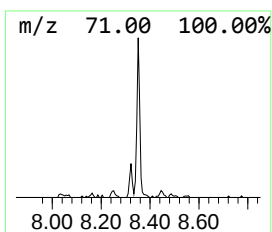
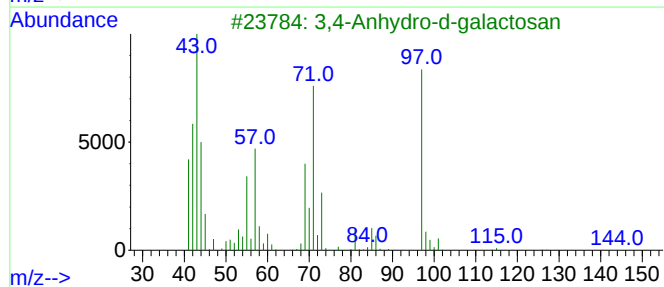
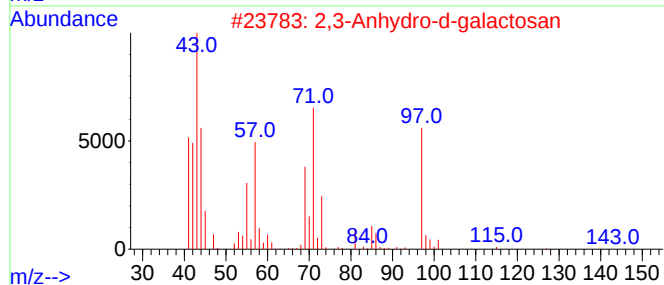
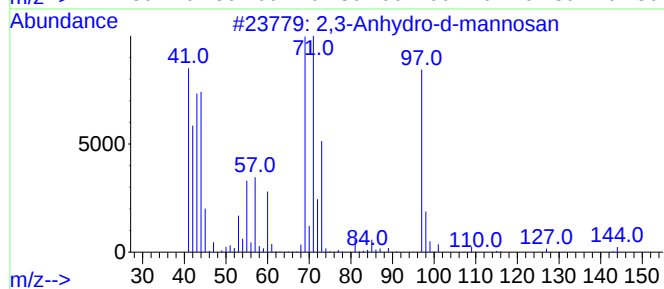
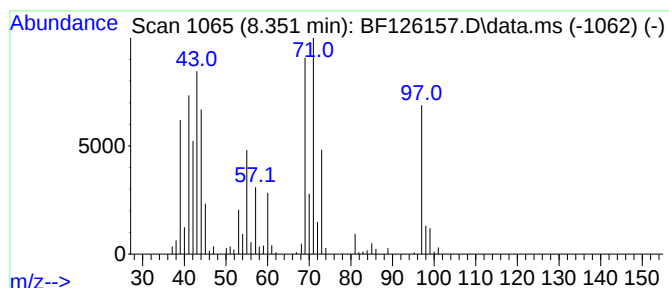
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,3-Anhydro-d-mannosan Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.351	6.62 ng	337409	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Anhydro-d-mannosan	144	C6H8O4	1000129-98-0	50
2			2,3-Anhydro-d-galactosan	144	C6H8O4	1000129-98-9	37
3			3,4-Anhydro-d-galactosan	144	C6H8O4	1000129-96-9	25
4			3-Hexenal	98	C6H10O	004440-65-7	14
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
Data File : BF126157.D
Acq On : 12 Nov 2021 15:23
Operator : JU/CG
Sample : M4572-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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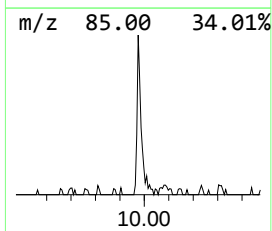
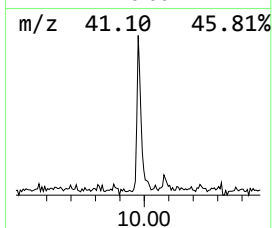
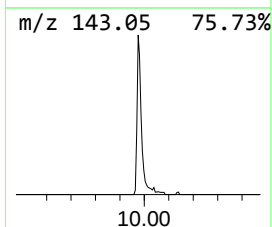
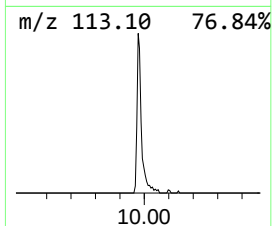
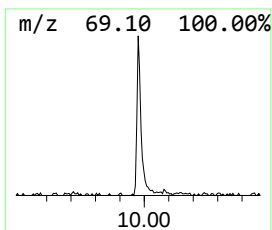
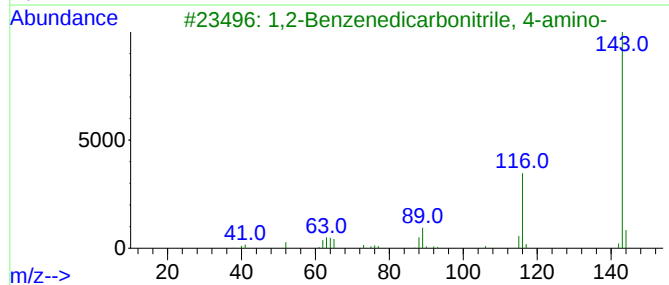
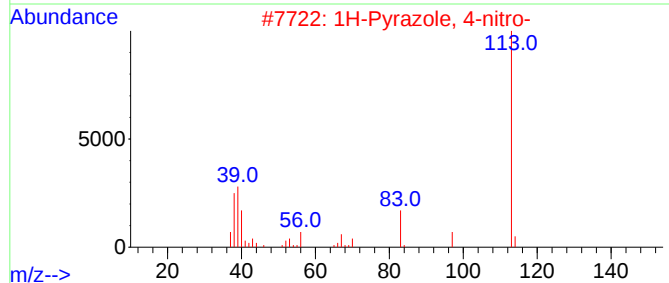
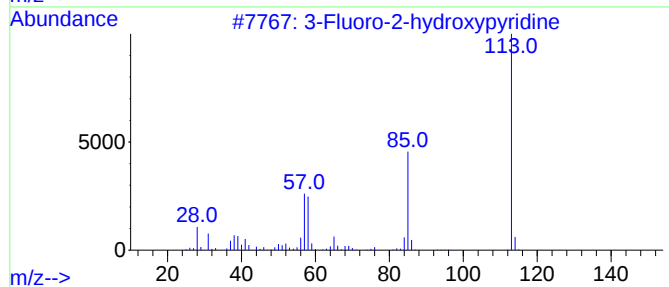
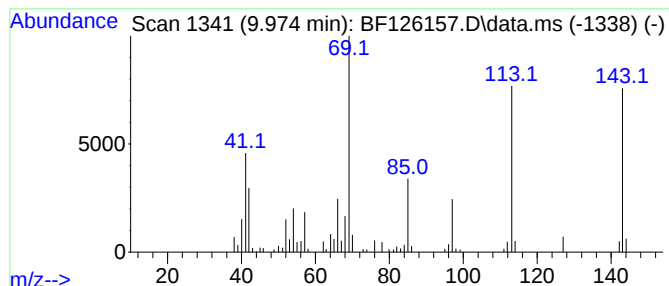
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.974 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.974	3.83 ng	240515	Acenaphthene-d10	9.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Fluoro-2-hydroxypyridine	113	C5H4FNO	001547-29-1	11
2			1H-Pyrazole, 4-nitro-	113	C3H3N3O2	002075-46-9	11
3			1,2-Benzenedicarbonitrile, 4-amino-	143	C8H5N3	056765-79-8	11
4			Thiazole, 4,5-dimethyl-	113	C5H7NS	003581-91-7	10
5			4-Fluoro-2-pyridone	113	C5H4FNO	096530-75-5	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
Data File : BF126157.D
Acq On : 12 Nov 2021 15:23
Operator : JU/CG
Sample : M4572-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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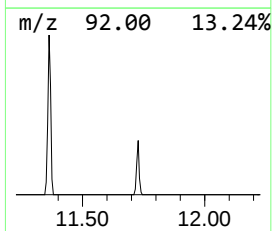
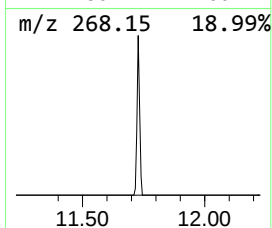
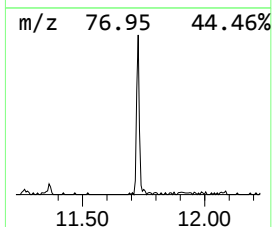
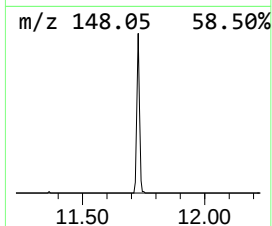
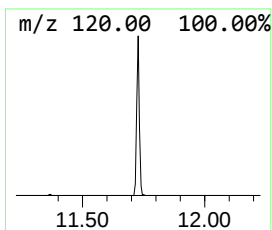
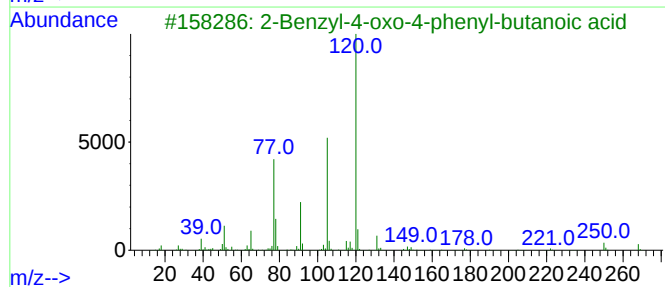
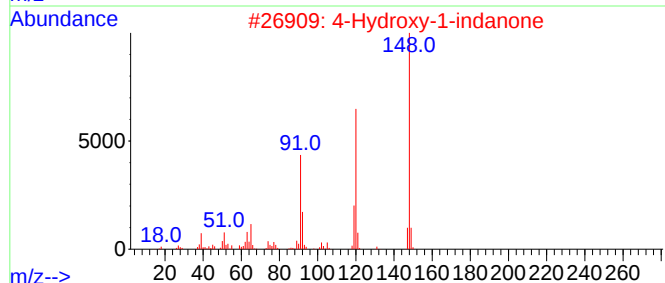
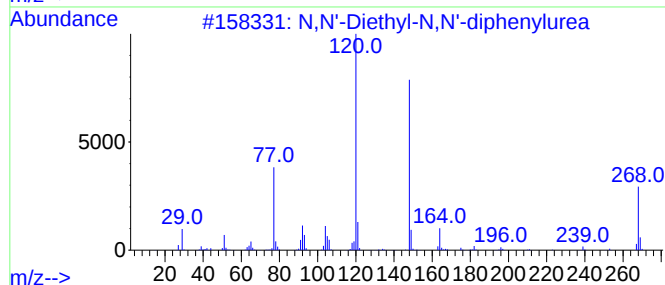
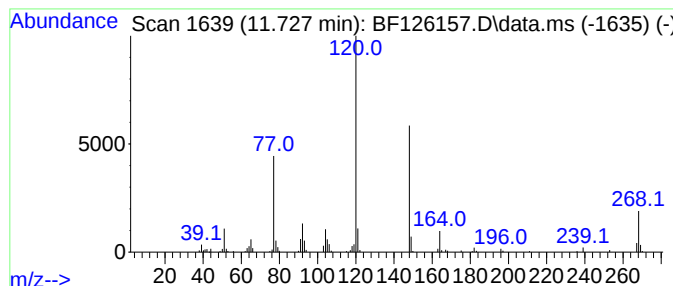
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 N,N'-Diethyl-N,N'-diphenylurea Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.727	2.95 ng	204117	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N,N'-Diethyl-N,N'-diphenylurea	268	C17H20N2O	000085-98-3	96
2			4-Hydroxy-1-indanone	148	C9H8O2	040731-98-4	50
3			2-Benzyl-4-oxo-4-phenyl-butanoic...	268	C17H16O3	104905-00-2	50
4			Aniline, N-(3-chloropropyl)-N-me...	183	C10H14ClN	1000380-56-8	50
5			4H-1-Benzopyran-4-one, 2,3-dihydro-	148	C9H8O2	000491-37-2	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
Data File : BF126157.D
Acq On : 12 Nov 2021 15:23
Operator : JU/CG
Sample : M4572-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

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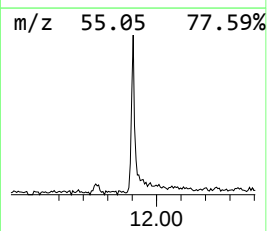
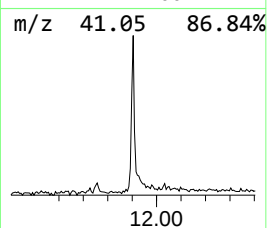
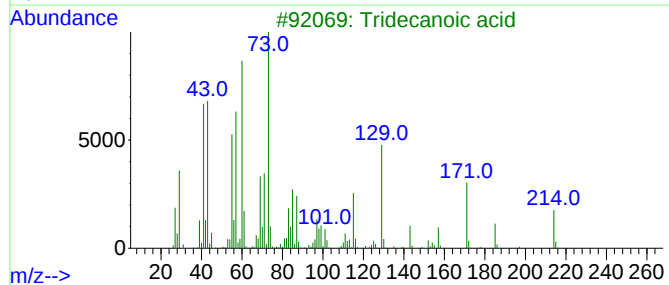
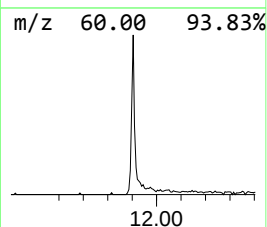
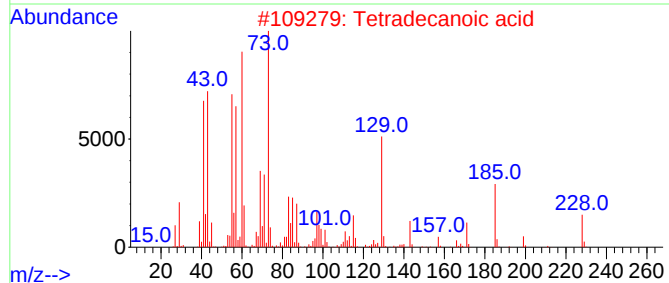
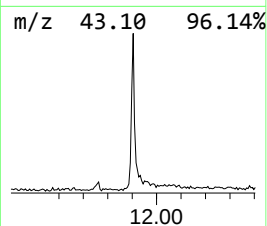
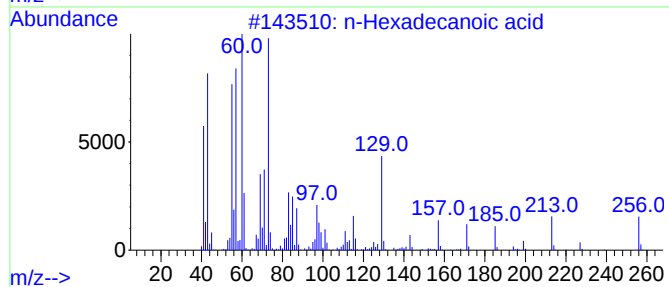
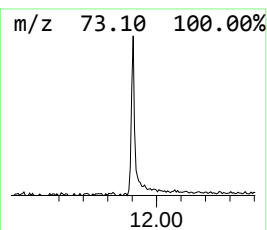
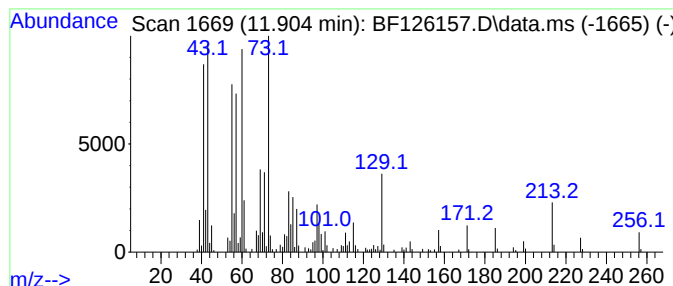
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	5.87 ng	405188	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Tridecanoic acid	214	C13H26O2	000638-53-9	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
Data File : BF126157.D
Acq On : 12 Nov 2021 15:23
Operator : JU/CG
Sample : M4572-06
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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
2-Pentanone, 4-...	5.051	57.5	ng	2271860	1	6.839	789544	20.0
unknown-5.181	5.181	2.7	ng	105787	1	6.839	789544	20.0
unknown5.404	5.404	3.9	ng	155482	1	6.839	789544	20.0
Methyl 2,5,8,11...	6.087	9.7	ng	382421	1	6.839	789544	20.0
1-Hexanol, 2-et...	6.904	7.5	ng	295908	1	6.839	789544	20.0
unknown7.722	7.722	15.1	ng	767930	2	8.128	1018790	20.0
Ethanol, 2-[2-(...	8.033	2.6	ng	131621	2	8.128	1018790	20.0
2,3-Anhydro-d-m...	8.351	6.6	ng	337409	2	8.128	1018790	20.0
unknown9.974	9.974	3.8	ng	240515	3	9.880	1257240	20.0
N,N'-Diethyl-N,...	11.727	3.0	ng	204117	4	11.363	1381600	20.0
n-Hexadecanoic ...	11.904	5.9	ng	405188	4	11.363	1381600	20.0