

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
 Data File : BF138276.D
 Acq On : 20 Jun 2024 22:12
 Operator : CG\JU
 Sample : P2955-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138276.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	9	15	21	rVB	3012941	3725993	76.52%	7.916%
2	3.387	217	221	237	rBV	107170	233765	4.80%	0.497%
3	3.969	310	320	326	rBV	52843	88062	1.81%	0.187%
4	5.098	509	512	518	rVB	297733	336103	6.90%	0.714%
5	5.504	570	581	584	rBV	4418977	3964715	81.42%	8.423%
6	5.904	644	649	654	rBV3	50694	65457	1.34%	0.139%
7	6.128	682	687	695	rBV4	48811	89702	1.84%	0.191%
8	6.416	733	736	738	rBV3	53199	61389	1.26%	0.130%
9	6.510	747	752	755	rBV	4131230	3809967	78.24%	8.094%
10	6.704	783	785	790	rBV2	267972	285876	5.87%	0.607%
11	6.881	812	815	819	rVB	2100681	1846350	37.92%	3.923%
12	6.939	822	825	829	rBV4	56281	65064	1.34%	0.138%
13	7.281	878	883	886	rBV3	70726	82235	1.69%	0.175%
14	7.445	906	911	914	rBV	2978659	2578914	52.96%	5.479%
15	7.475	914	916	920	rVB	94212	81295	1.67%	0.173%
16	7.522	920	924	928	rVB4	47582	66401	1.36%	0.141%
17	7.581	928	934	938	rBV3	38732	69156	1.42%	0.147%
18	7.692	950	953	958	rVB	187596	169298	3.48%	0.360%
19	8.104	1020	1023	1027	rBV4	58215	70354	1.44%	0.149%
20	8.163	1030	1033	1036	rVV	2944762	2421038	49.72%	5.144%
21	8.186	1036	1037	1040	rVV	182363	107914	2.22%	0.229%
22	8.222	1040	1043	1046	rVB	107342	87683	1.80%	0.186%
23	8.475	1083	1086	1095	rVB	384817	406411	8.35%	0.863%
24	8.580	1101	1104	1107	rBV	136415	134727	2.77%	0.286%
25	8.751	1130	1133	1136	rBV	160477	120975	2.48%	0.257%
26	8.875	1152	1154	1157	rVB	136824	96037	1.97%	0.204%
27	8.975	1168	1171	1174	rBV	98057	76865	1.58%	0.163%
28	9.157	1199	1202	1204	rBV	78208	62462	1.28%	0.133%
29	9.239	1212	1216	1219	rBV	6237006	4869427	100.00%	10.345%
30	9.316	1226	1229	1232	rBV	405254	374375	7.69%	0.795%
31	9.498	1257	1260	1265	rBV5	58023	96325	1.98%	0.205%
32	9.575	1271	1273	1275	rVB2	95210	72410	1.49%	0.154%
33	9.627	1279	1282	1286	rBV2	221012	253259	5.20%	0.538%
34	9.692	1289	1293	1295	rBV4	82611	104956	2.16%	0.223%
35	9.733	1298	1300	1303	rBV4	78788	74076	1.52%	0.157%
36	9.786	1306	1309	1311	rBV3	216348	215081	4.42%	0.457%

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Peak Location: TOP

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

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37	9.804	1311	1312	1314	rVB	97971	67069	1.38%	0.142%
38	9.827	1314	1316	1318	rBV	200529	149320	3.07%	0.317%
39	9.922	1325	1332	1335	rBV	2895780	2721045	55.88%	5.781%
40	9.957	1336	1338	1342	rVB3	82816	97438	2.00%	0.207%
41	10.016	1344	1348	1353	rBV	1817217	2445548	50.22%	5.196%
42	10.233	1383	1385	1387	rBV2	87563	92880	1.91%	0.197%
43	10.257	1387	1389	1392	rVB3	174093	154227	3.17%	0.328%
44	10.327	1398	1401	1403	rBV2	214160	199689	4.10%	0.424%
45	10.345	1403	1404	1407	rVB	112315	72106	1.48%	0.153%
46	10.457	1421	1423	1432	rBV8	108195	231045	4.74%	0.491%
47	10.704	1461	1465	1471	rBV	2778732	2534320	52.05%	5.384%
48	10.833	1483	1487	1490	rBV	390134	420811	8.64%	0.894%
49	11.404	1581	1584	1587	rBV	2607668	2162352	44.41%	4.594%
50	11.427	1587	1588	1594	rVB	298061	228191	4.69%	0.485%
51	11.933	1670	1674	1683	rVB2	804326	938986	19.28%	1.995%
52	12.715	1805	1807	1810	rBV2	292724	294379	6.05%	0.625%
53	12.992	1850	1854	1857	rBV	3375660	3274942	67.26%	6.958%
54	14.045	2030	2033	2036	rBV	1853470	1575459	32.35%	3.347%
55	15.521	2281	2284	2287	rVB	1126436	1201307	24.67%	2.552%
56	16.680	2478	2481	2498	rVB	450495	944158	19.39%	2.006%

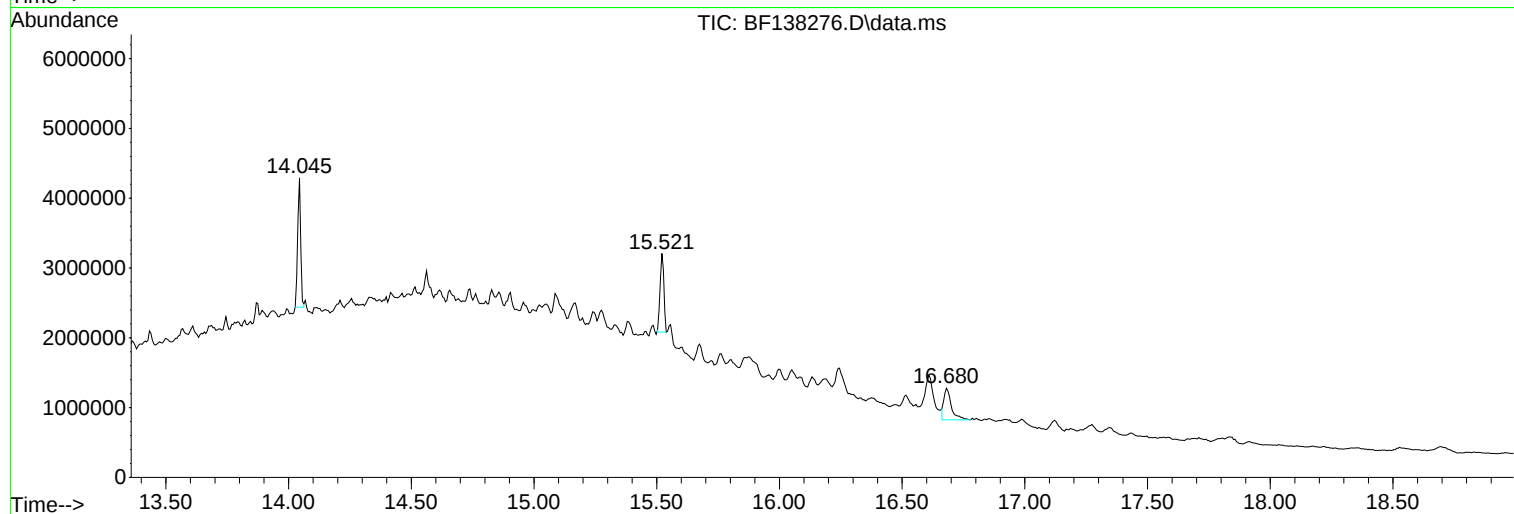
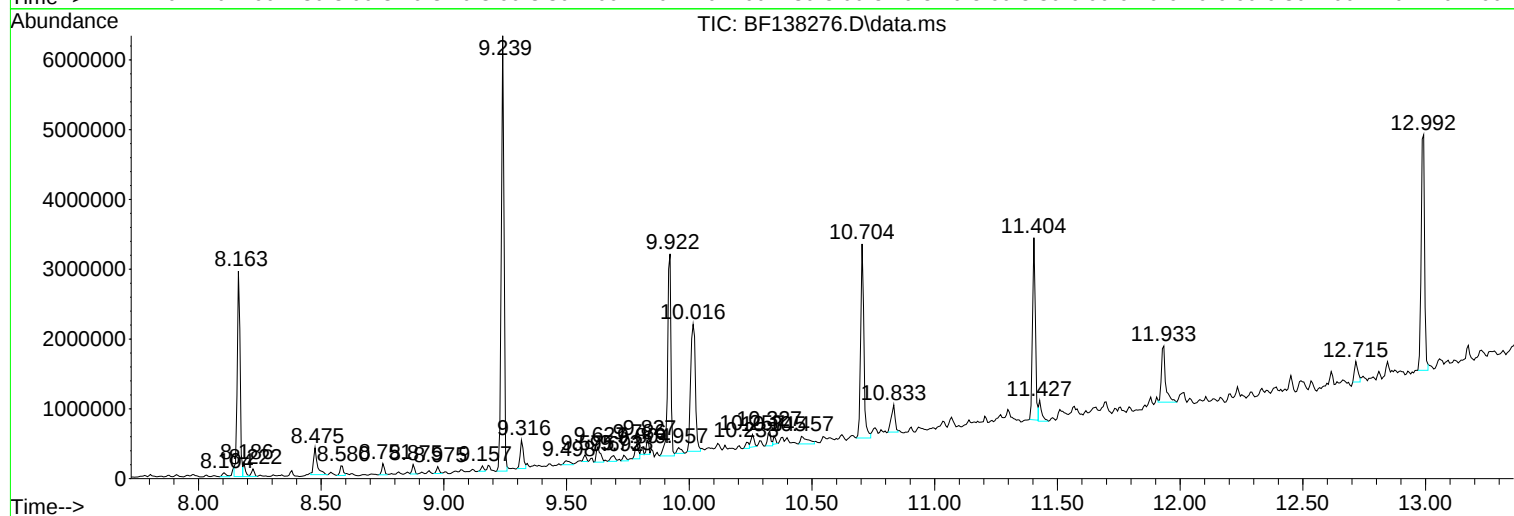
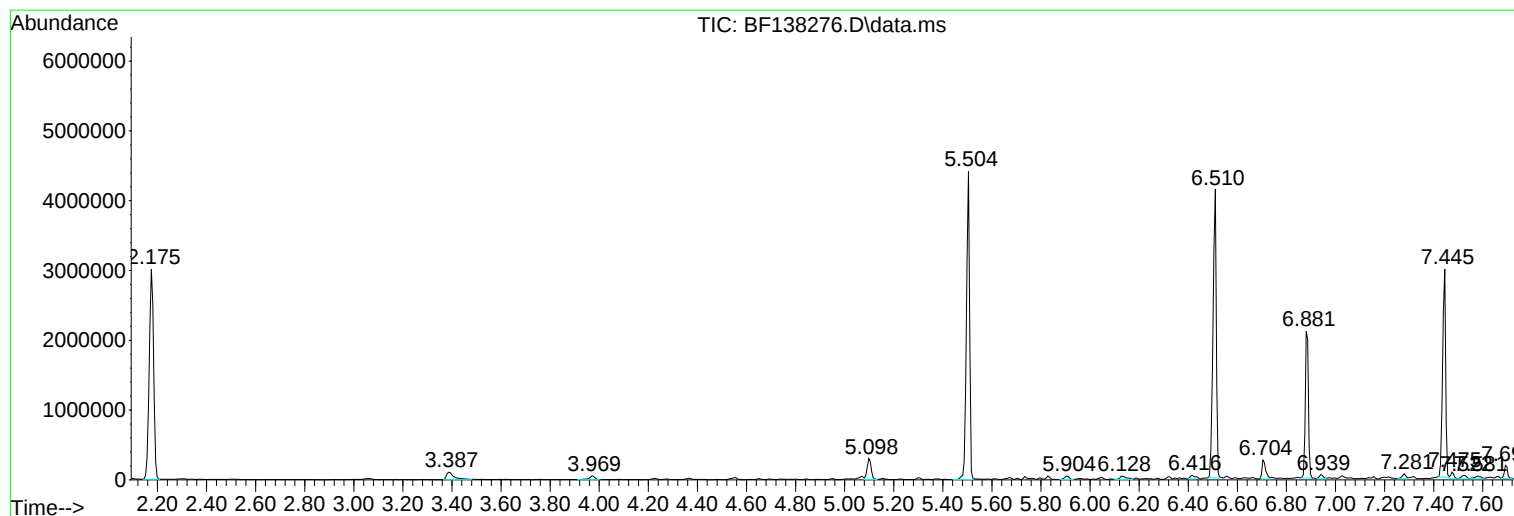
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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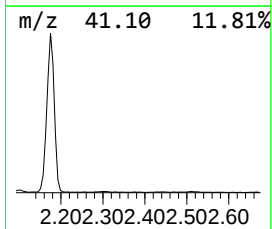
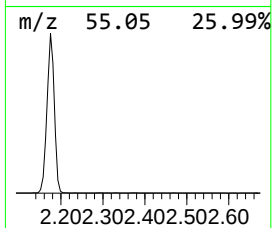
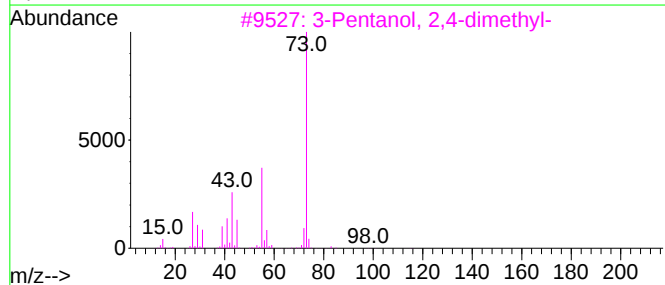
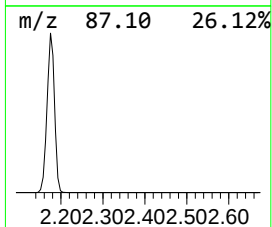
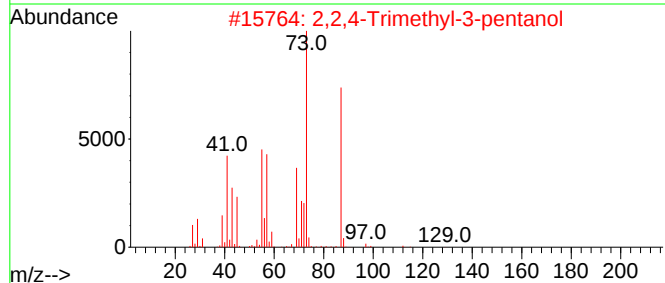
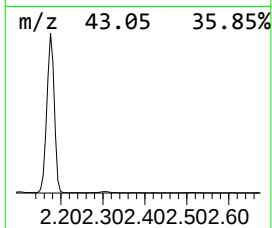
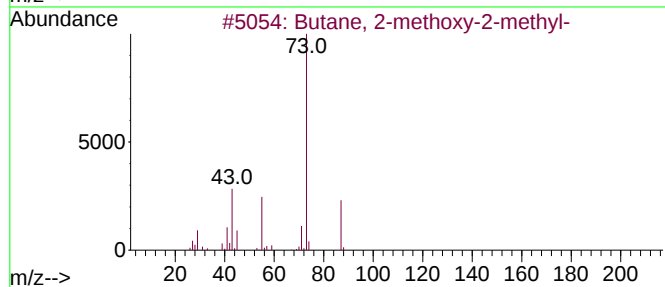
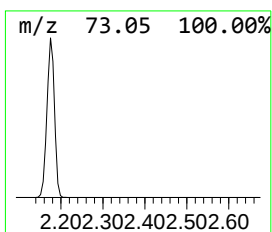
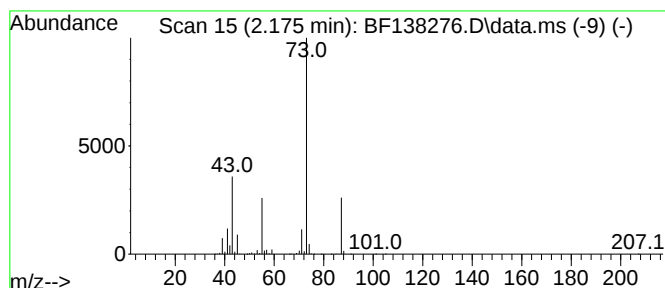
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.175	40.36 ng	3725990	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23



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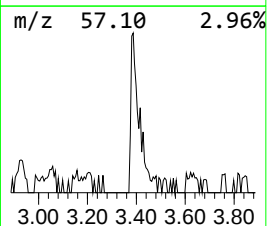
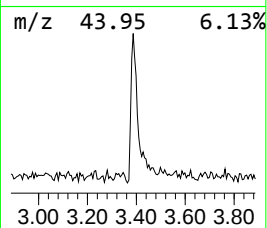
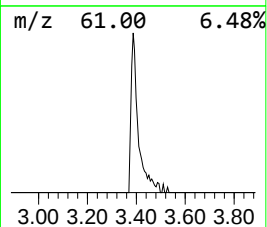
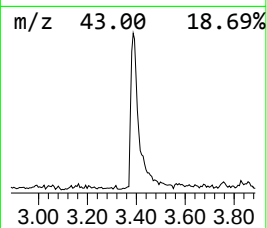
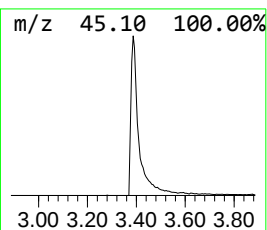
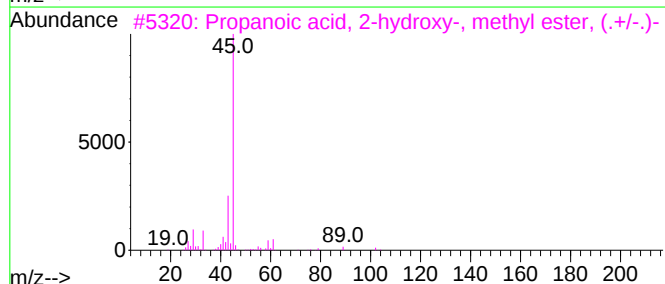
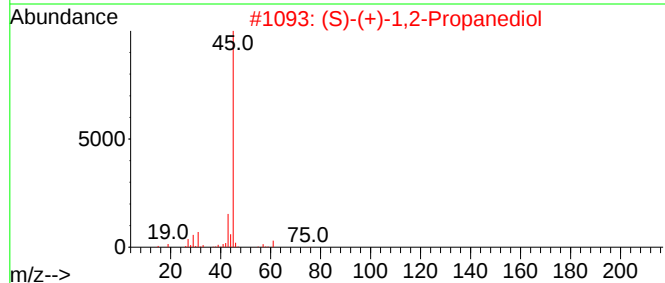
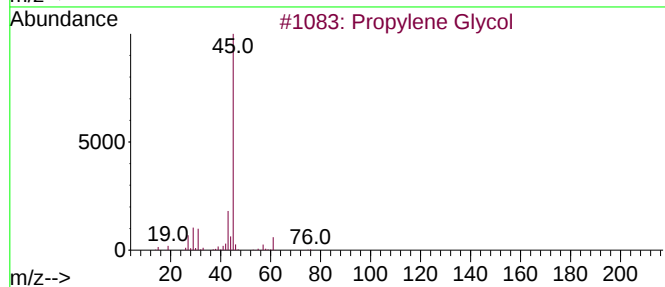
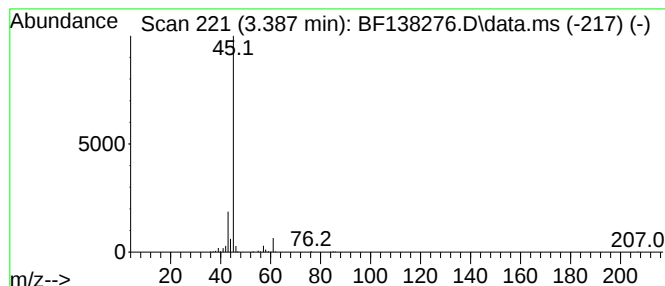
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	2.53 ng	233765	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	32
5			2-Pentanol	88	C5H12O	006032-29-7	9



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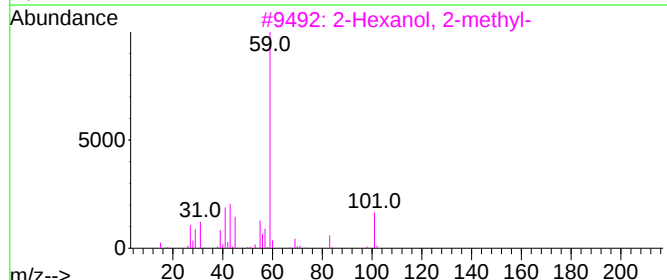
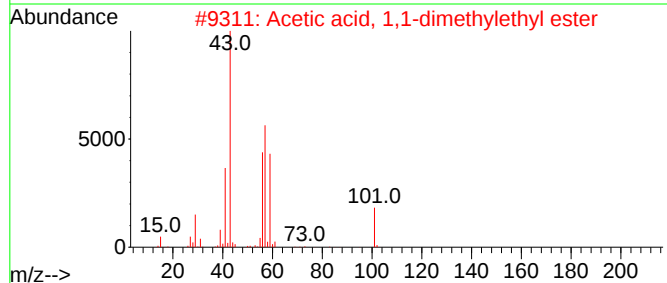
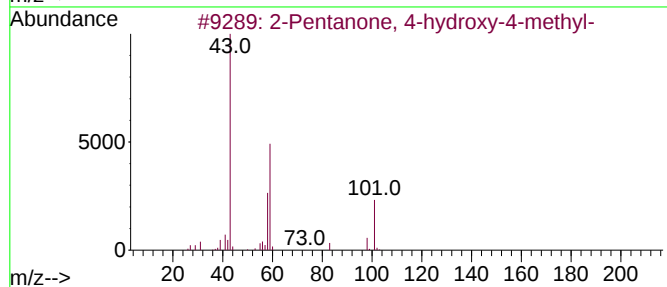
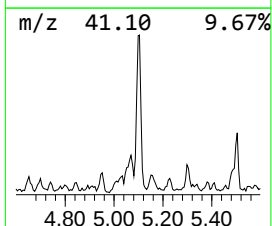
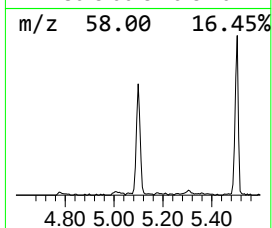
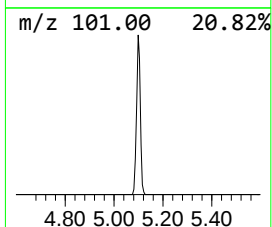
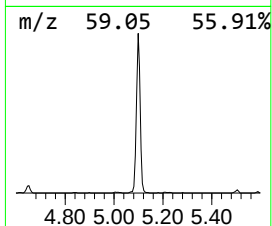
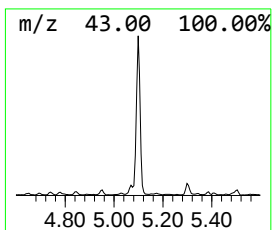
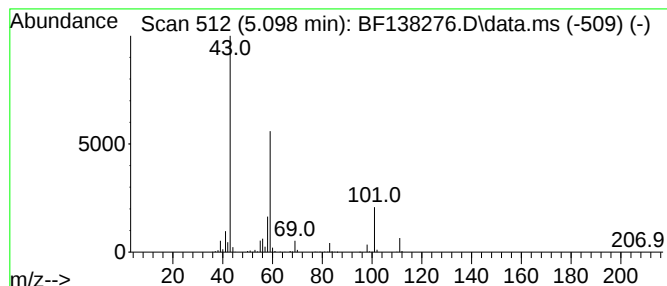
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.098	3.64 ng	336103	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	17
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17



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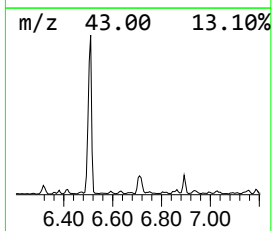
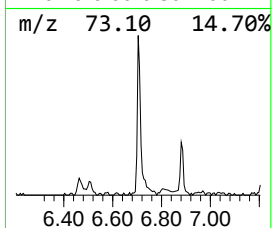
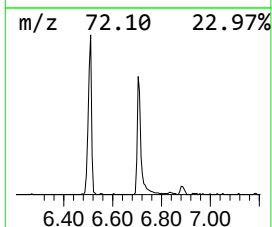
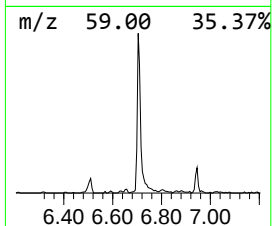
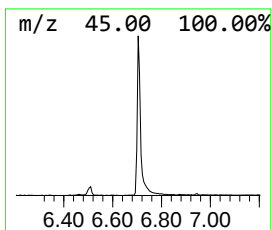
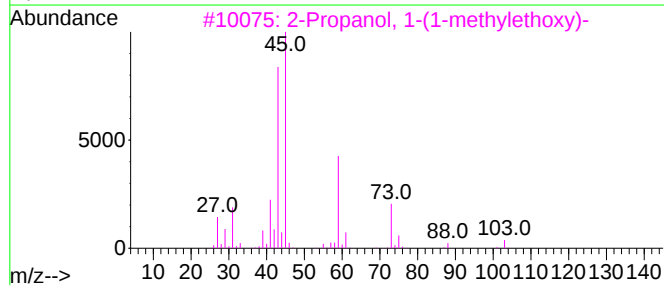
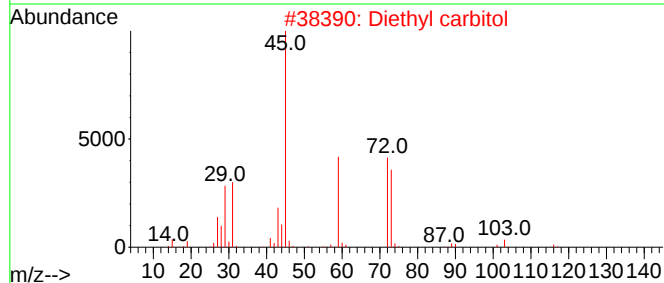
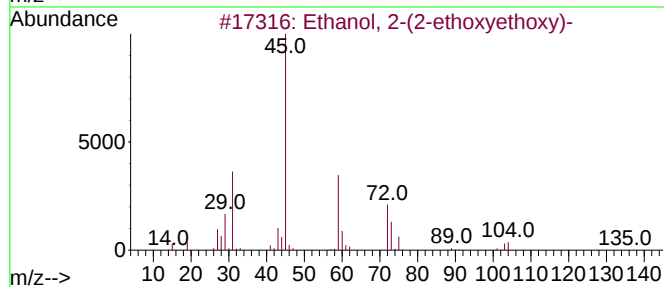
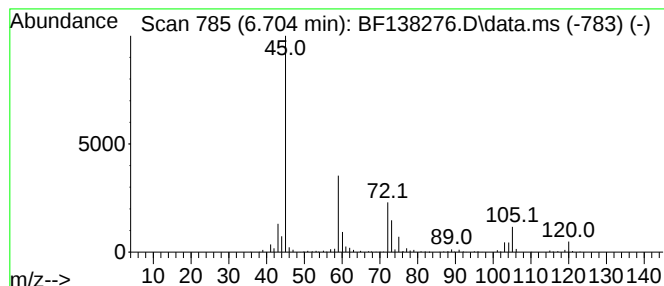
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.704	3.10 ng	285876	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	78
2			Diethyl carbitol	162	C8H18O3	000112-36-7	64
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	42
4			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	40
5			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	38



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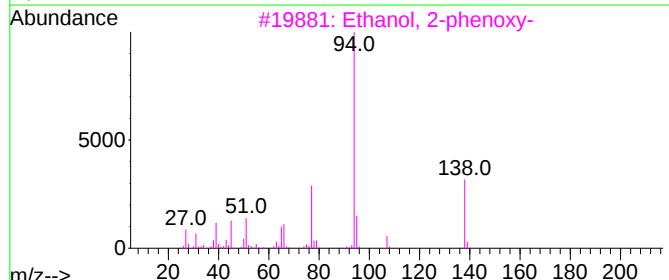
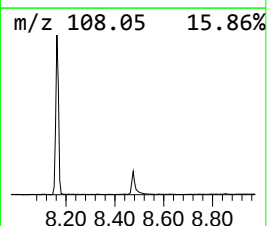
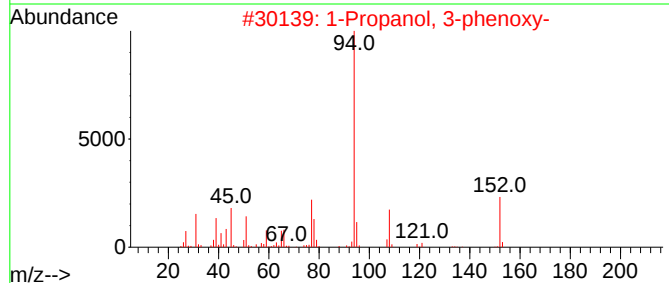
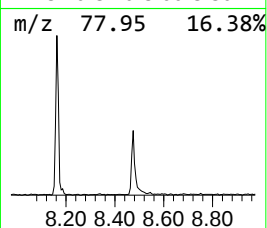
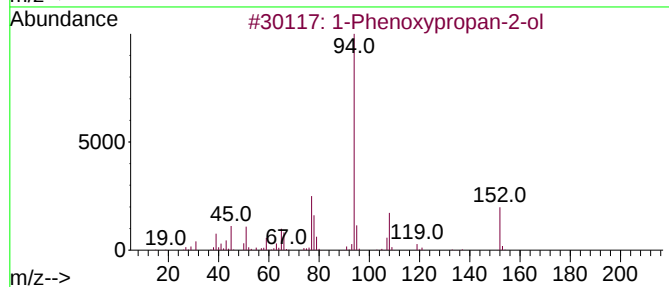
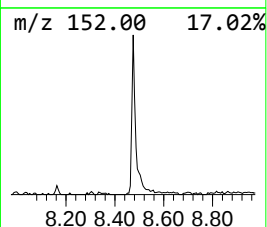
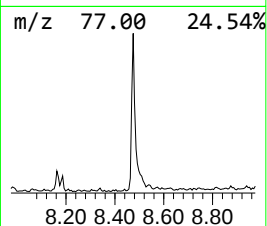
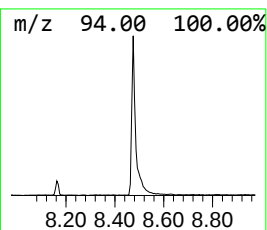
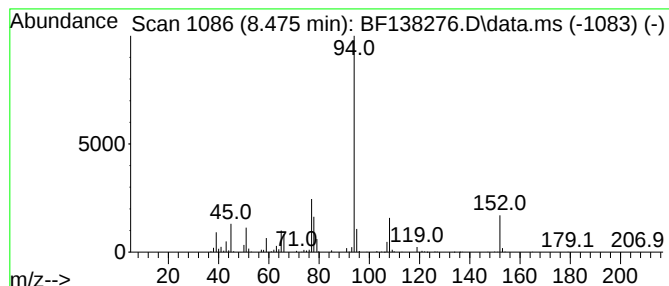
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.475	3.36 ng	406411	Naphthalene-d8	8.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	90
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, sec-butyl phenyl ...	194	C11H14O3	013183-17-0	59
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138276.D
Acq On : 20 Jun 2024 22:12
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

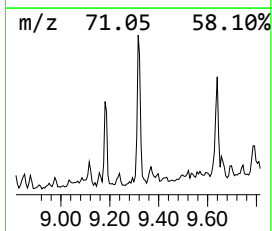
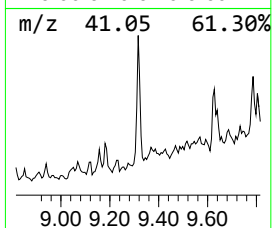
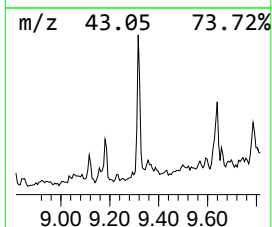
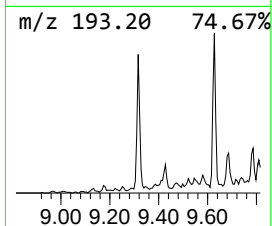
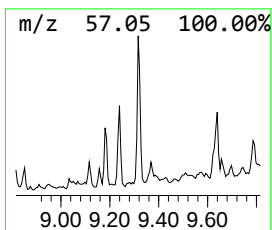
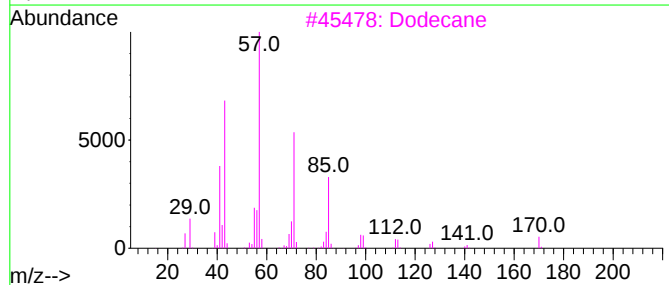
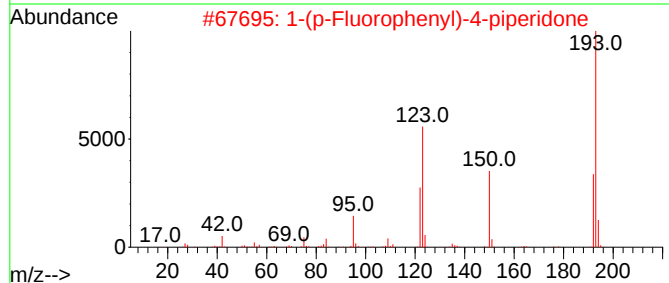
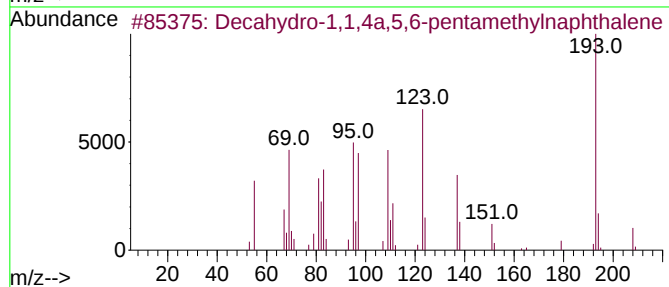
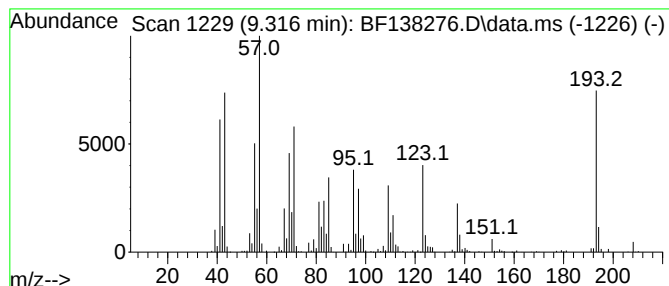
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.316	2.75 ng	374375	Acenaphthene-d10	9.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	95
2		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
3		Dodecane	170	C12H26	000112-40-3	25
4		2H-Spiro[1-benzofuran-3,2'-[1,3]...	193	C10H11NO3	1000387-33-4	18
5		2-Anthracenamine	193	C14H11N	000613-13-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138276.D
Acq On : 20 Jun 2024 22:12
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

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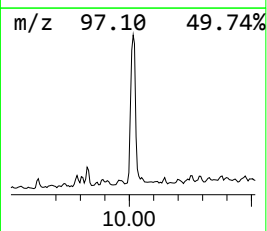
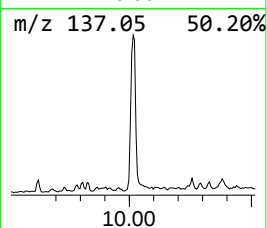
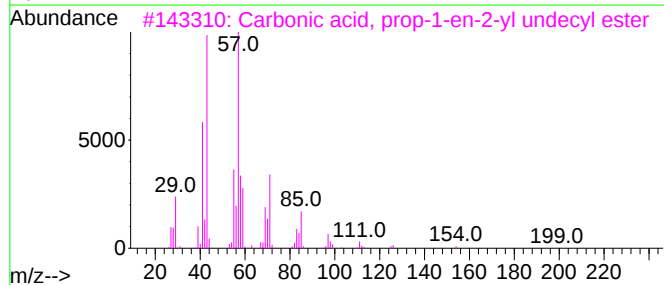
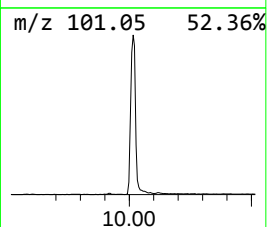
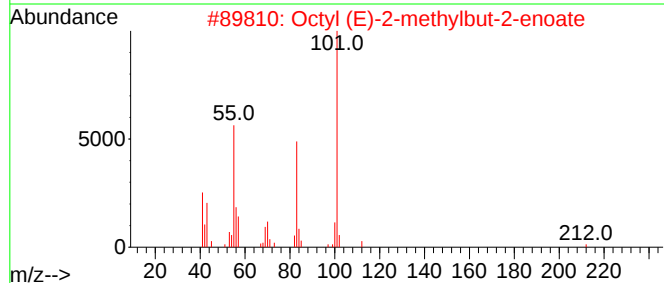
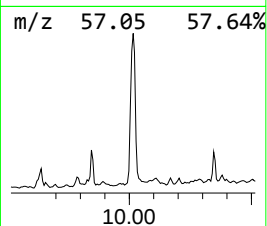
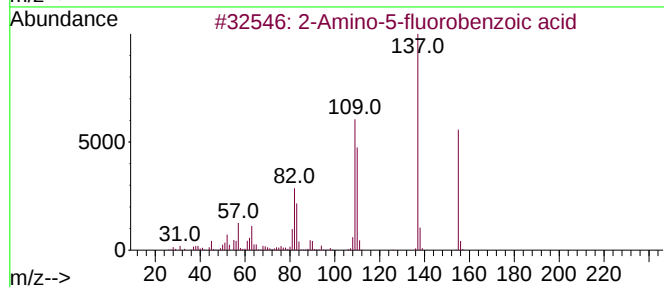
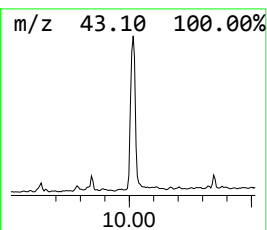
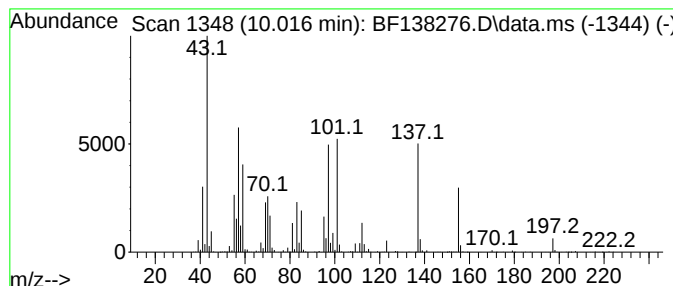
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown10.016 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.016	17.98 ng	2445550	Acenaphthene-d10	9.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Amino-5-fluorobenzoic acid	155	C7H6FN02	000446-08-2	10
2		Octyl (E)-2-methylbut-2-enoate	212	C13H24O2	1000373-71-2	10
3		Carbonic acid, prop-1-en-2-yl un...	256	C15H28O3	1000382-90-6	10
4		Anthralic acid, 6-fluoro-	155	C7H6FN02	000434-76-4	10
5		Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138276.D
Acq On : 20 Jun 2024 22:12
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

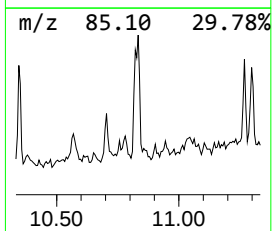
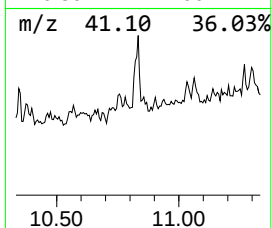
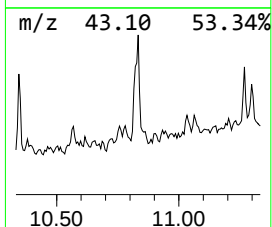
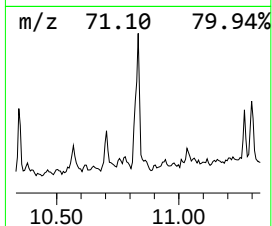
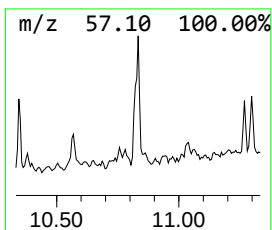
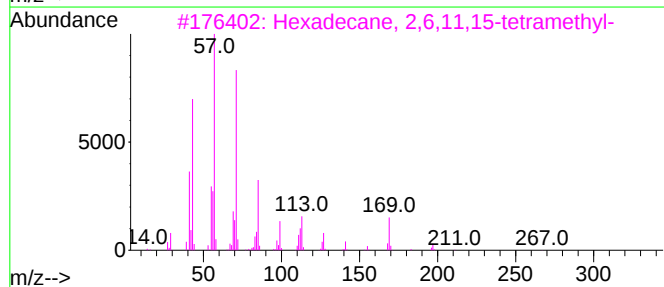
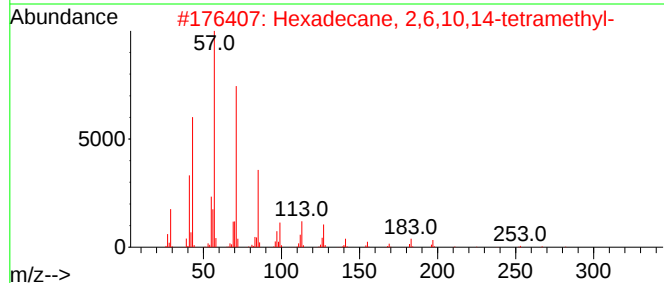
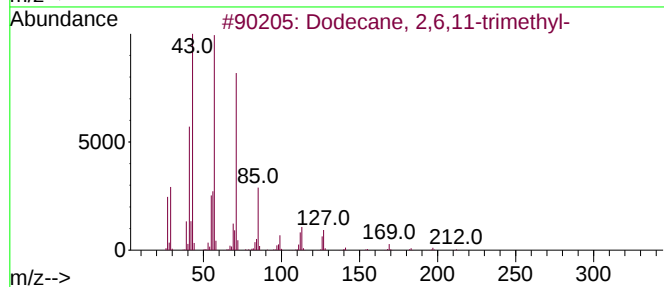
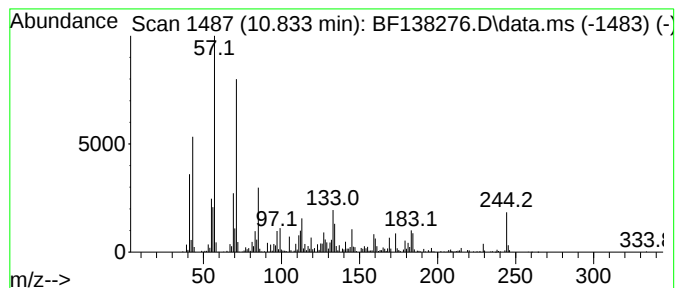
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecane, 2,6,11-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.833	3.89 ng	420811	Phenanthrene-d10	11.404	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	83
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	58
3	Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	58
4	Decane, 2-methyl-	156	C11H24	006975-98-0	53
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138276.D
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Sample : P2955-05
Misc :
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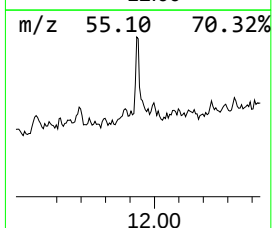
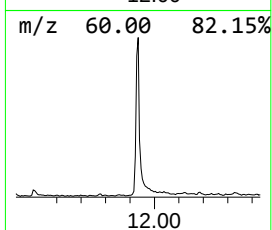
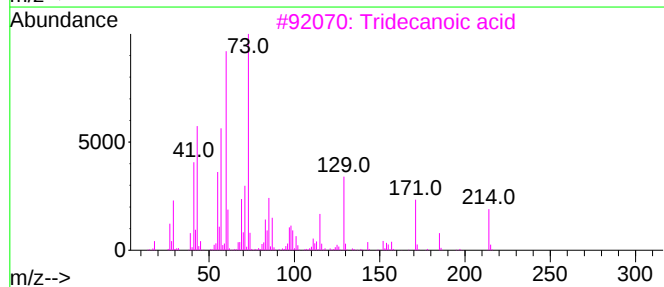
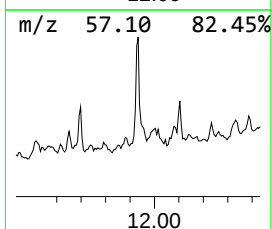
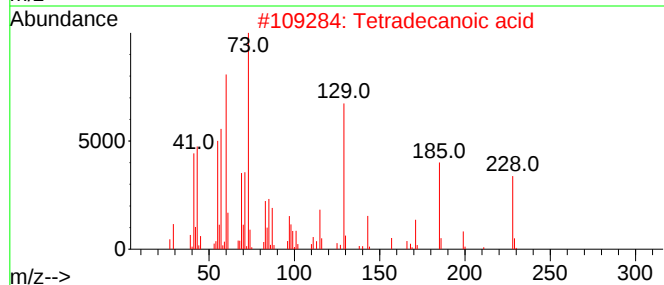
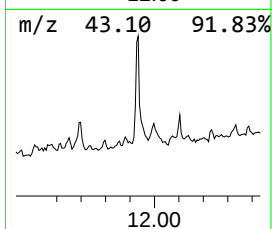
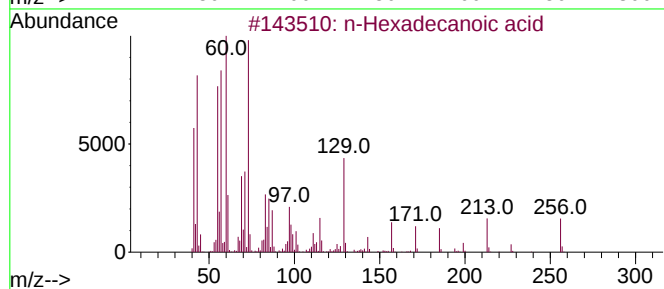
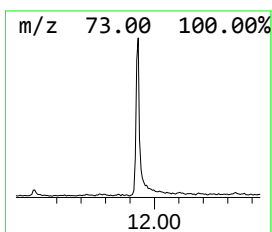
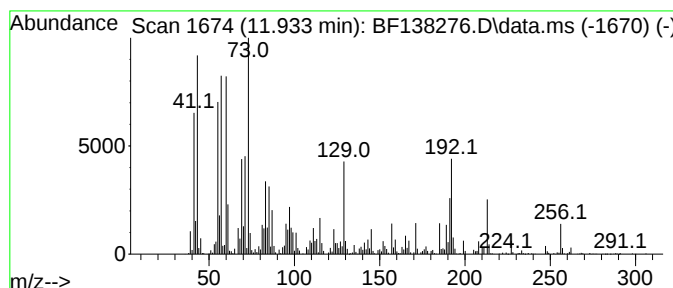
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.933	8.68 ng	938986	Phenanthrene-d10	11.404	
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	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Octadecanoic acid	284	C18H36O2	000057-11-4	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138276.D
Acq On : 20 Jun 2024 22:12
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

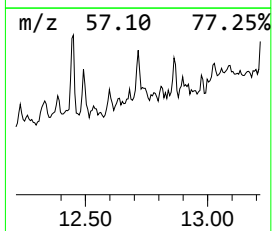
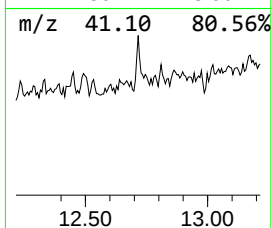
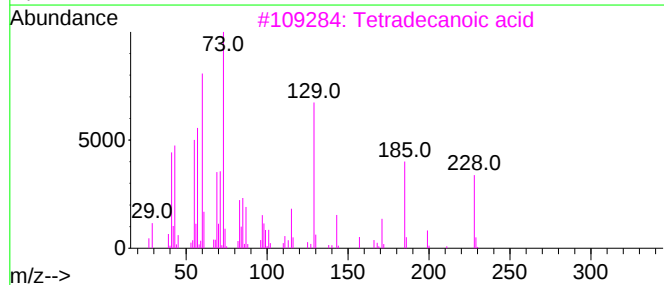
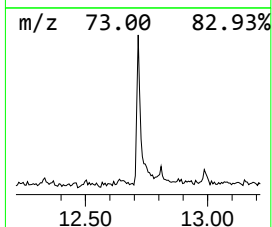
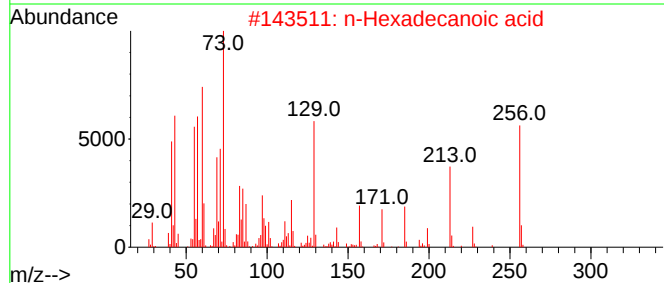
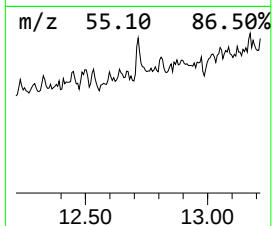
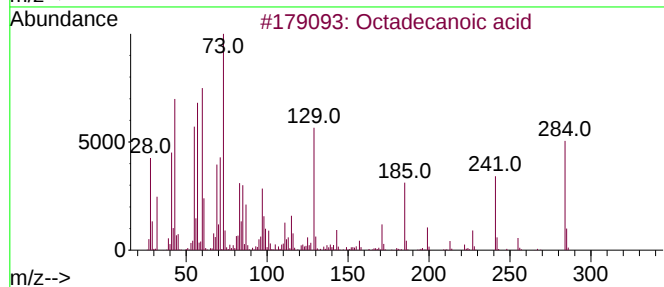
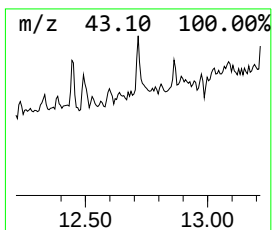
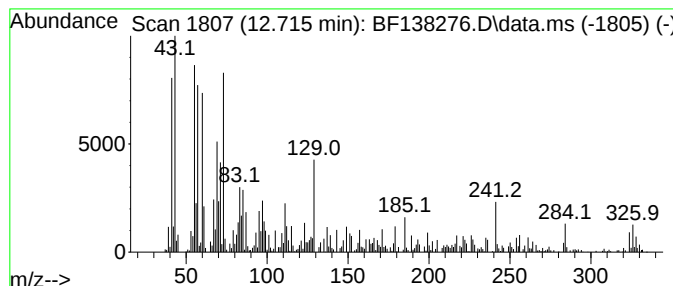
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.72 ng	294379	Phenanthrene-d10	11.404

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4		Heneicosanoic acid	326	C21H42O2	002363-71-5	89
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
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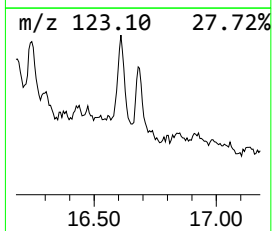
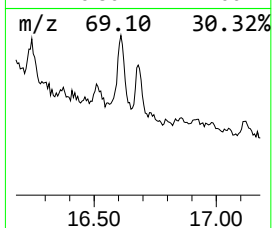
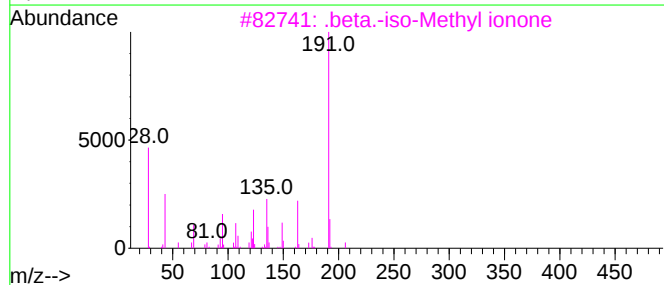
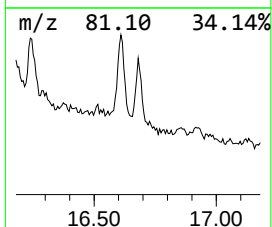
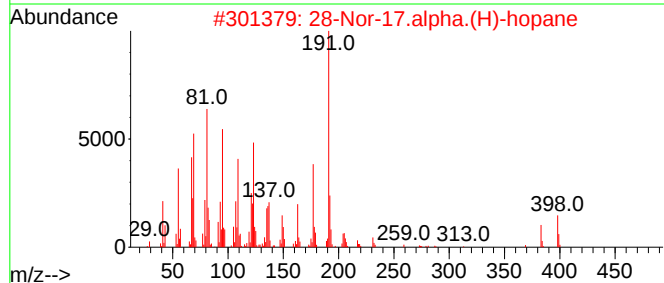
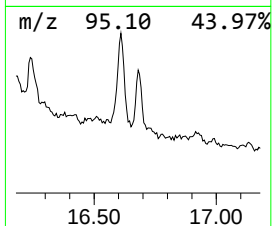
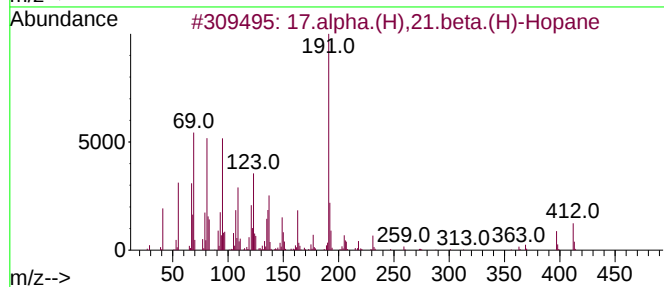
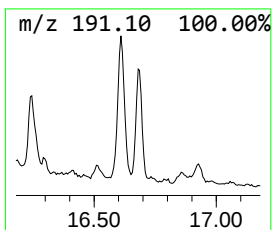
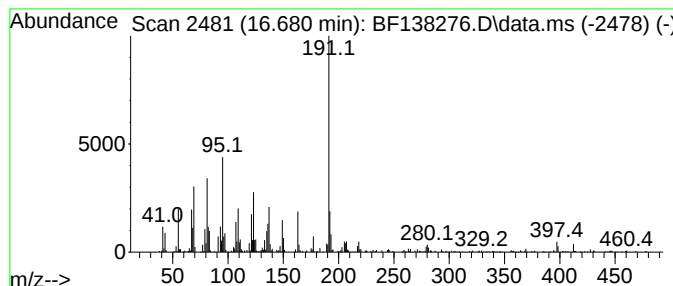
Instrument :
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ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.680	15.72 ng	944158	Perylene-d12		15.521	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	17.alpha.(H),21.beta.(H)-Hopane		412	C30H52	013849-96-2	83
2	28-Nor-17.alpha.(H)-hopane		398	C29H50	053584-60-4	70
3	.beta.-iso-Methyl ionone		206	C14H22O	1000285-40-2	46
4	1-Penten-3-one, 1-(2,6,6-trimeth...		206	C14H22O	000127-43-5	46
5	Propenamide, 3-(3,4-dimethoxyphe...		313	C18H19NO4	339165-72-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062024\
Data File : BF138276.D
Acq On : 20 Jun 2024 22:12
Operator : CG\JU
Sample : P2955-05
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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...	2.175	40.4	ng	3725990	1	6.886	1846350	20.0
Propylene Glycol	3.387	2.5	ng	233765	1	6.886	1846350	20.0
2-Pentanone, 4-...	5.098	3.6	ng	336103	1	6.886	1846350	20.0
Ethanol, 2-(2-e...	6.704	3.1	ng	285876	1	6.886	1846350	20.0
1-Phenoxypropan...	8.475	3.4	ng	406411	2	8.163	2421040	20.0
Decahydro-1,1,4...	9.316	2.8	ng	374375	3	9.922	2721050	20.0
unknown10.016	10.016	18.0	ng	2445550	3	9.922	2721050	20.0
Dodecane, 2,6,1...	10.833	3.9	ng	420811	4	11.404	2162350	20.0
n-Hexadecanoic ...	11.933	8.7	ng	938986	4	11.404	2162350	20.0
Octadecanoic acid	12.716	2.7	ng	294379	4	11.404	2162350	20.0
17.alpha.(H),21...	16.680	15.7	ng	944158	6	15.521	1201310	20.0