

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
 Data File : BF133997.D
 Acq On : 27 Jun 2023 18:28
 Operator : CG\JU
 Sample : 03398-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133997.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	5	11	19	rVB	1173517	1471166	25.27%	4.151%
2	5.093	508	511	518	rBV	64323	78614	1.35%	0.222%
3	5.487	573	578	581	rBV	2176204	1959435	33.65%	5.528%
4	6.487	743	748	751	rBV	2081605	1956513	33.60%	5.520%
5	6.851	806	810	814	rBV	730142	572137	9.83%	1.614%
6	7.410	901	905	909	rBV	1298223	1242703	21.34%	3.506%
7	8.128	1024	1027	1031	rBV	824613	677268	11.63%	1.911%
8	9.151	1198	1201	1204	rBV	116201	97894	1.68%	0.276%
9	9.210	1207	1211	1214	rVV	2216713	1889442	32.45%	5.331%
10	9.281	1220	1223	1227	rBV3	178491	205710	3.53%	0.580%
11	9.481	1255	1257	1260	rBV3	80106	105188	1.81%	0.297%
12	9.592	1274	1276	1278	rBV	819300	768449	13.20%	2.168%
13	9.651	1281	1286	1290	rVV7	192121	314723	5.40%	0.888%
14	9.704	1293	1295	1300	rVB3	143031	134377	2.31%	0.379%
15	9.751	1300	1303	1306	rBV2	520624	622655	10.69%	1.757%
16	9.798	1309	1311	1314	rVB	1160702	966921	16.61%	2.728%
17	9.839	1315	1318	1320	rBV3	274582	280274	4.81%	0.791%
18	9.875	1320	1324	1325	rBV2	524885	702737	12.07%	1.983%
19	9.892	1325	1327	1330	rVB	739127	577746	9.92%	1.630%
20	9.928	1330	1333	1336	rBV3	302803	415492	7.14%	1.172%
21	9.998	1343	1345	1349	rBV4	223381	307454	5.28%	0.867%
22	10.151	1368	1371	1374	rBV2	535522	678084	11.65%	1.913%
23	10.210	1379	1381	1383	rBV3	407453	466516	8.01%	1.316%
24	10.263	1388	1390	1393	rVV2	487530	565284	9.71%	1.595%
25	10.304	1393	1397	1400	rVV2	1362958	1298331	22.30%	3.663%
26	10.557	1437	1440	1443	rVB	1741643	1569784	26.96%	4.429%
27	10.692	1460	1463	1465	rBV	937815	802861	13.79%	2.265%
28	10.833	1481	1487	1489	rBV	4830058	5822817	100.00%	16.429%
29	11.298	1563	1566	1570	rVB	2790517	2818007	48.40%	7.951%
30	11.651	1624	1626	1629	rVB	1065423	833453	14.31%	2.352%
31	12.992	1852	1854	1862	rVB	1449151	1515714	26.03%	4.277%
32	14.027	2027	2030	2032	rBV	441131	422098	7.25%	1.191%
33	14.051	2032	2034	2037	rVB	451347	359404	6.17%	1.014%
34	14.774	2153	2157	2162	rVB2	444489	716840	12.31%	2.023%
35	14.921	2177	2182	2185	rBV	1729177	1916515	32.91%	5.407%
36	15.551	2286	2289	2294	rVB	259416	310014	5.32%	0.875%

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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-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

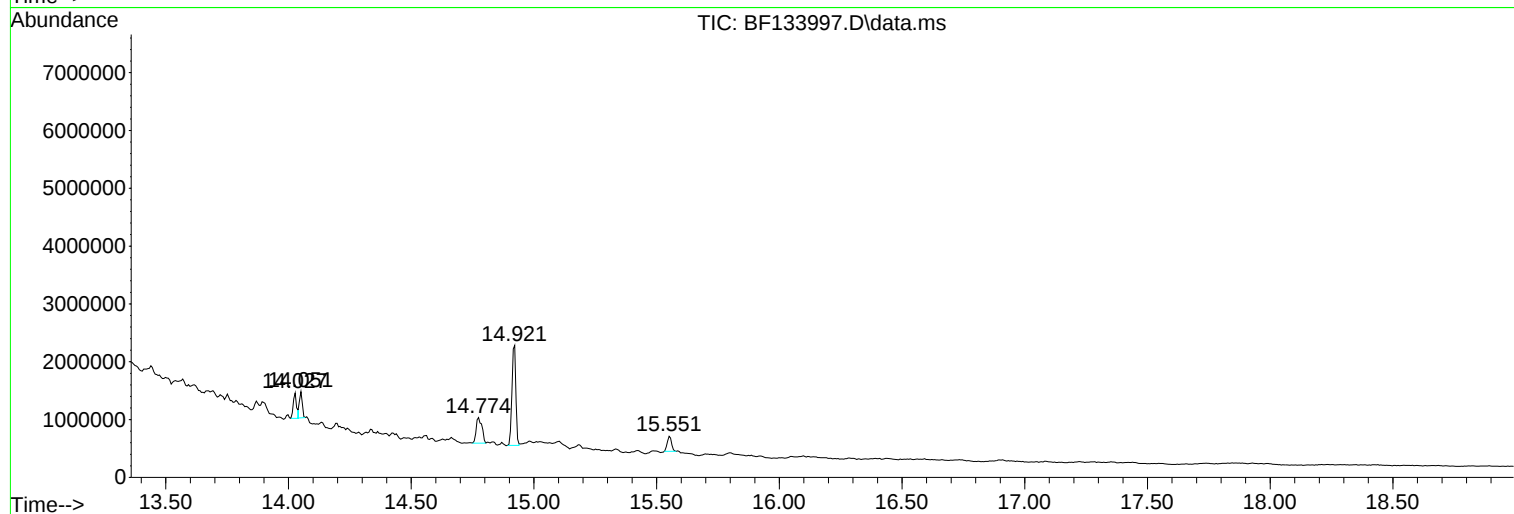
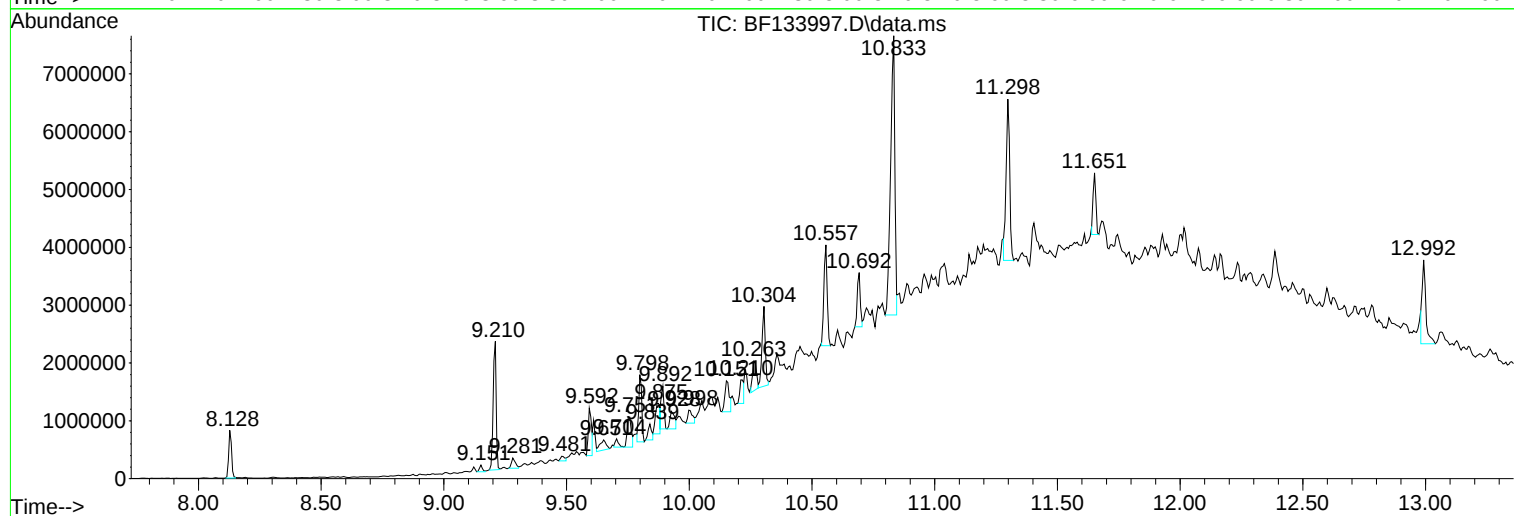
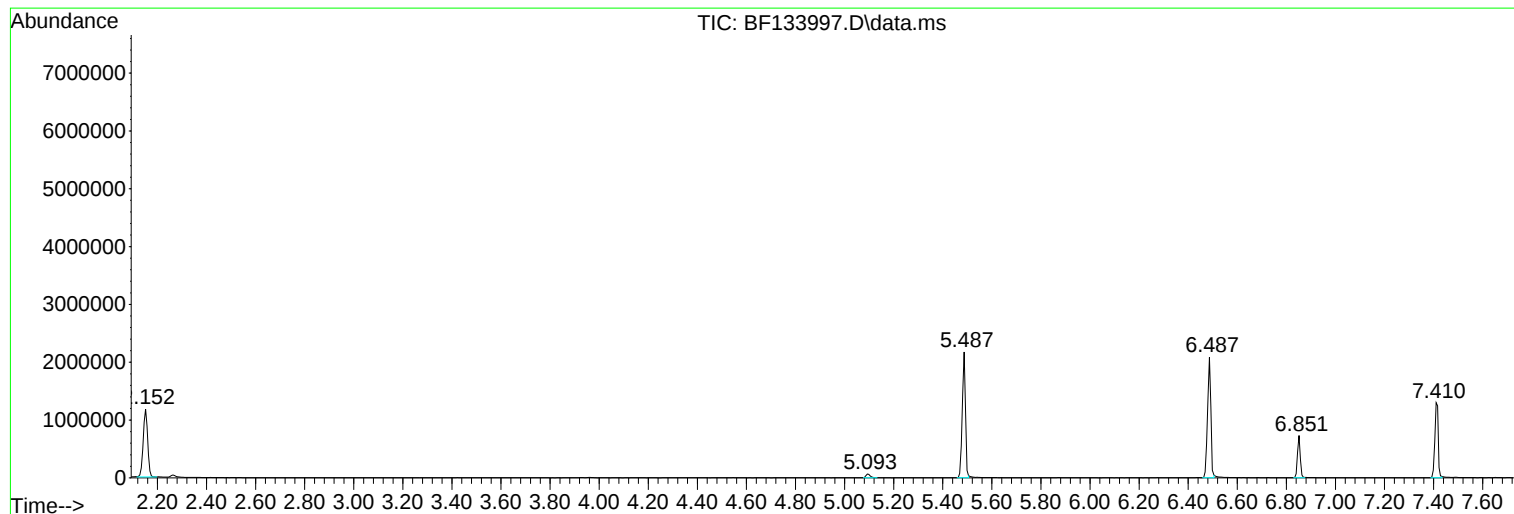
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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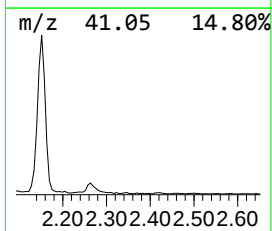
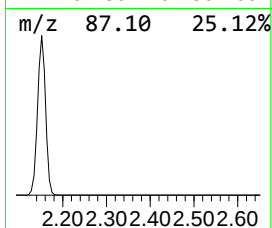
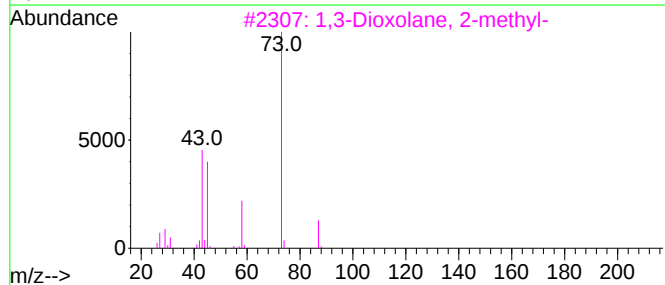
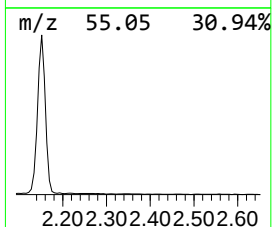
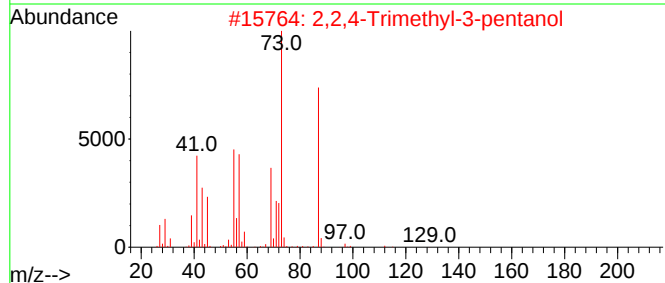
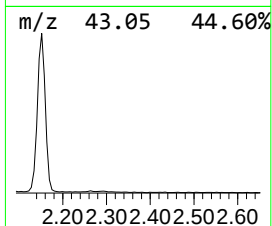
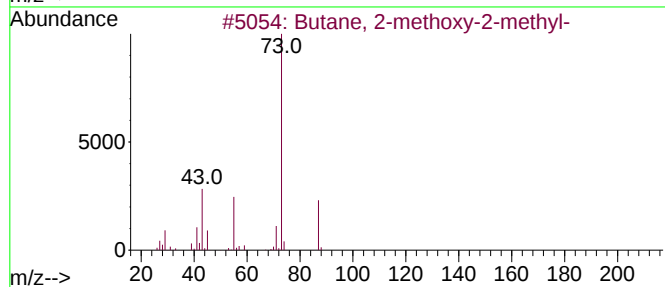
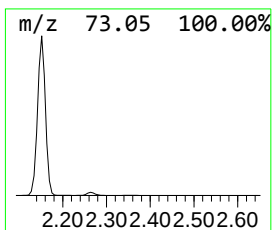
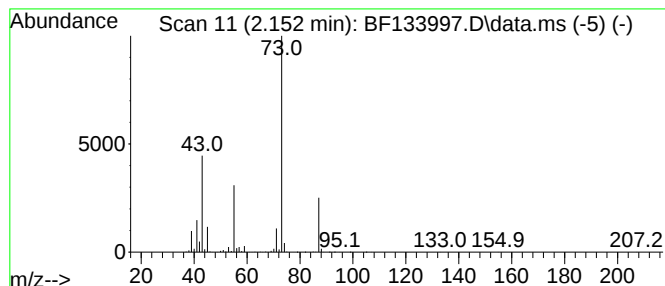
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	51.43 ng	1471170	1,4-Dichlorobenzene-d4	6.851

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			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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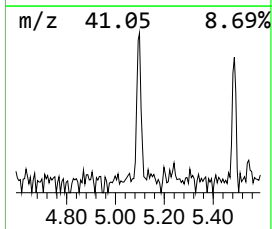
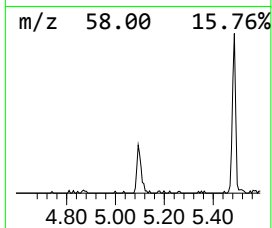
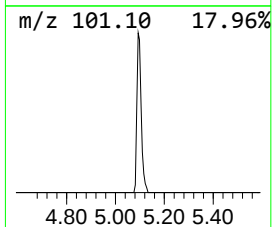
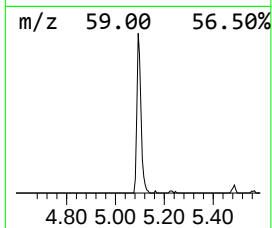
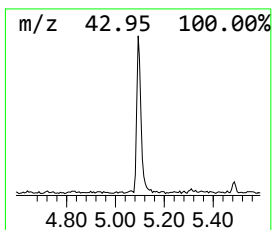
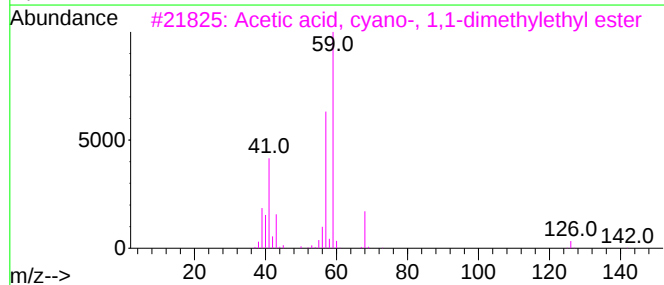
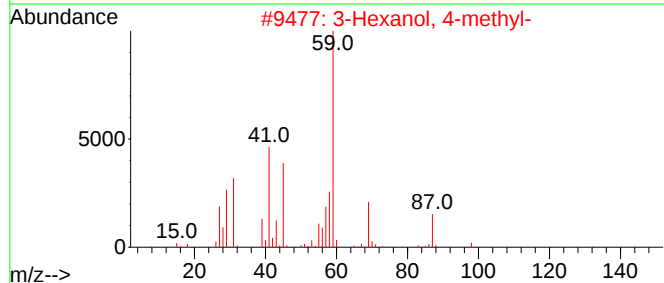
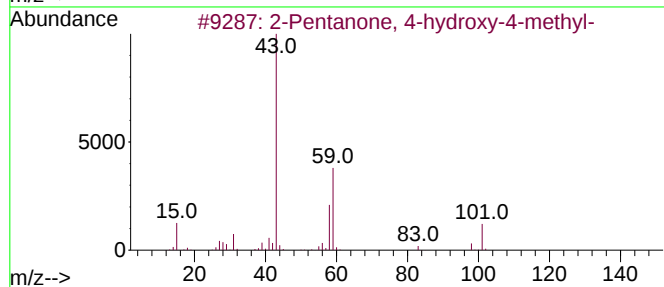
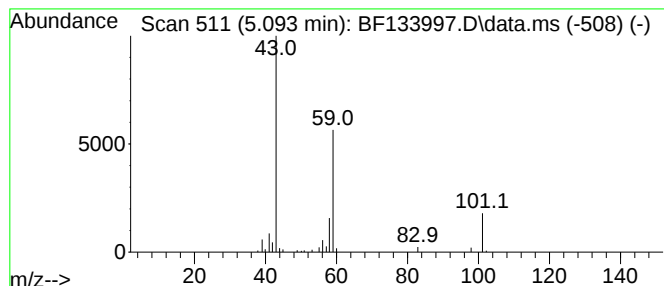
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	2.75 ng	78614	1,4-Dichlorobenzene-d4	6.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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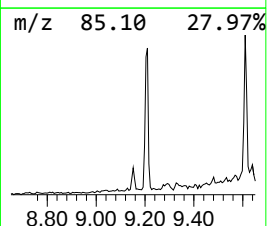
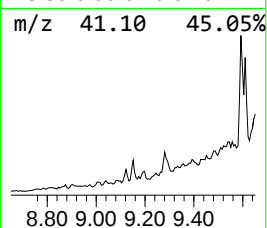
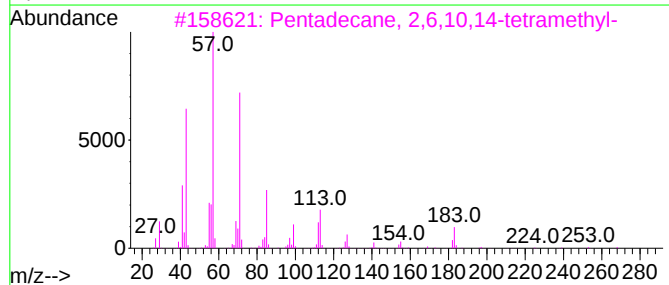
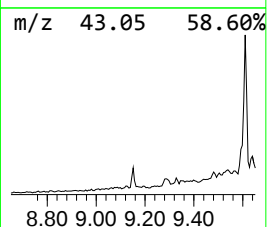
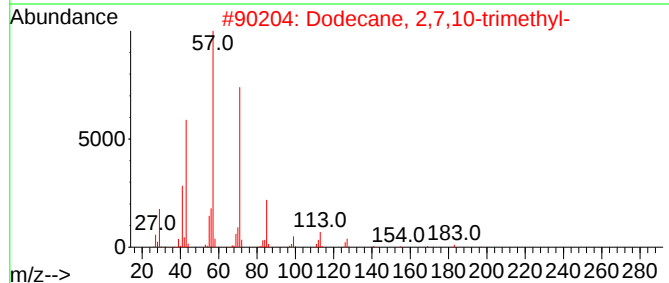
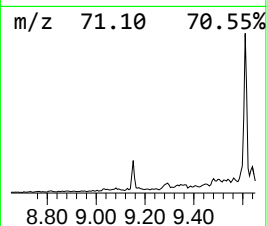
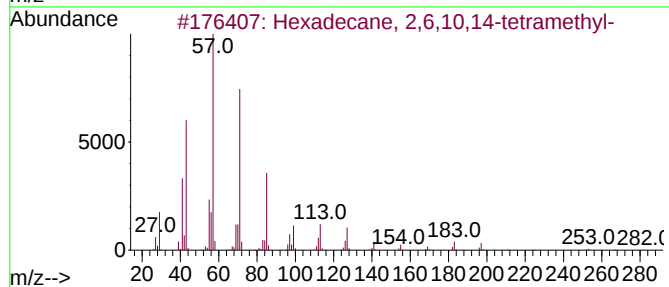
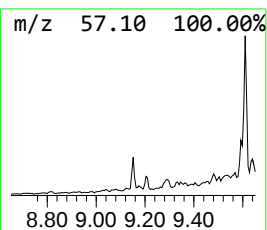
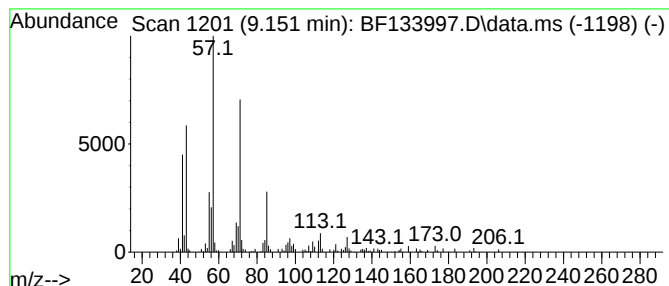
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecane, 2,6,10,14-tetra... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.151	3.39 ng	97894	Acenaphthene-d10	9.892

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
2		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3		Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	80
4		Octane, 2-methyl-	128	C9H20	003221-61-2	72
5		Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	64



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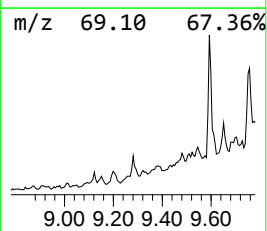
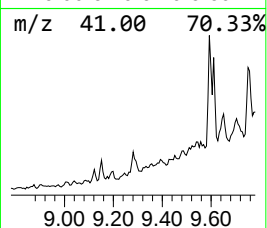
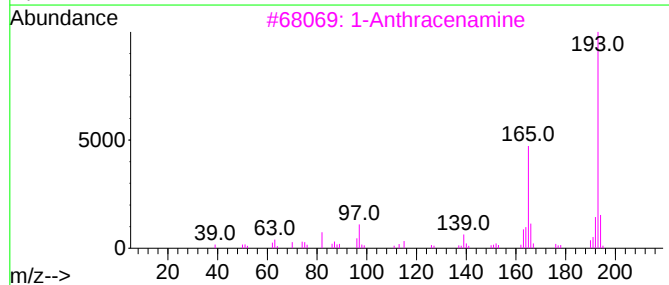
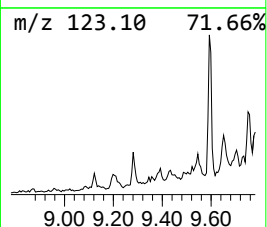
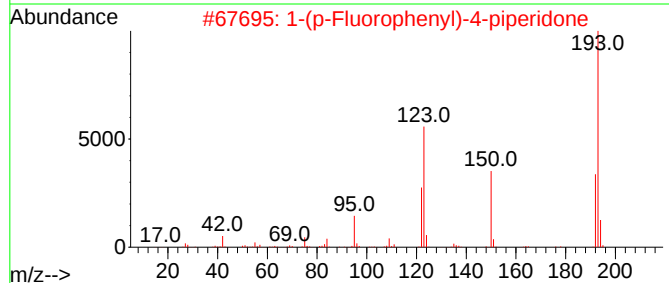
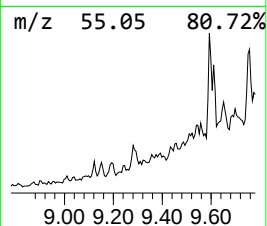
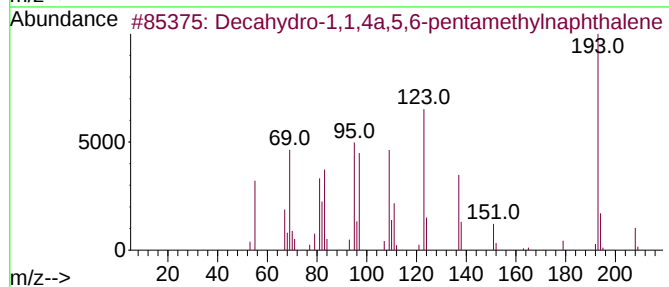
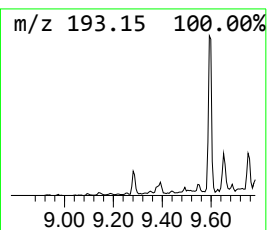
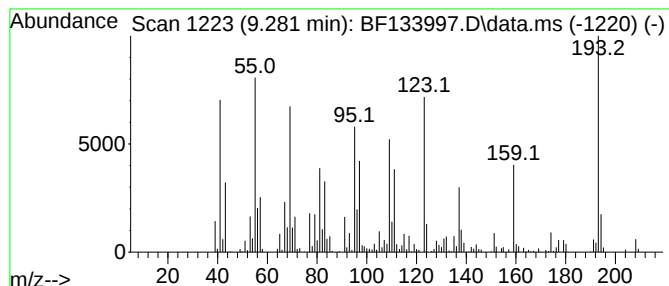
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Peak Number 4 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.281	7.12 ng	205710	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	50
2			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	27
3			1-Anthracenamine	193	C14H11N	000610-49-1	27
4			2-Anthracenamine	193	C14H11N	000613-13-8	22
5			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	18



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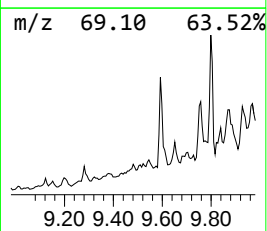
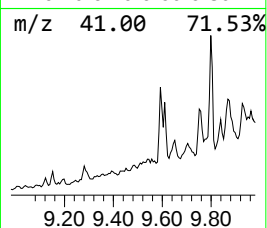
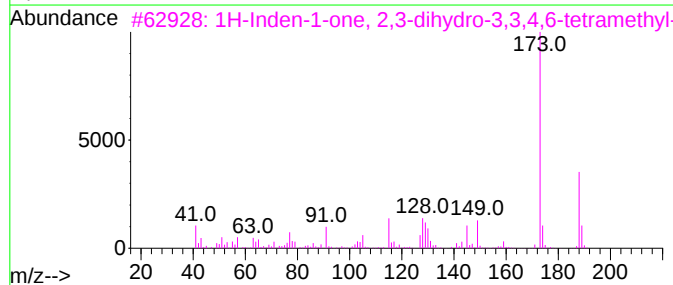
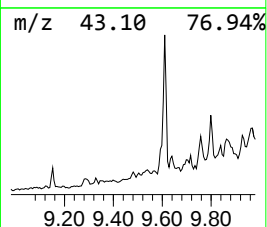
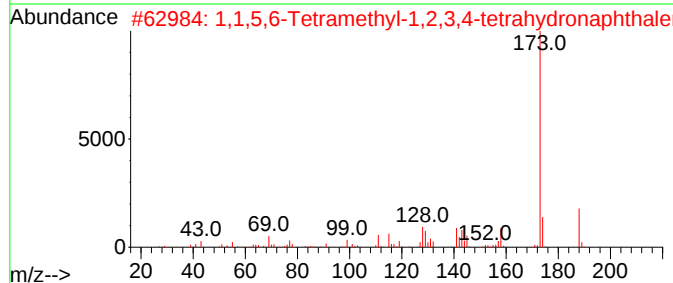
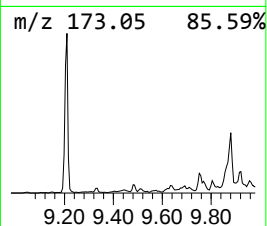
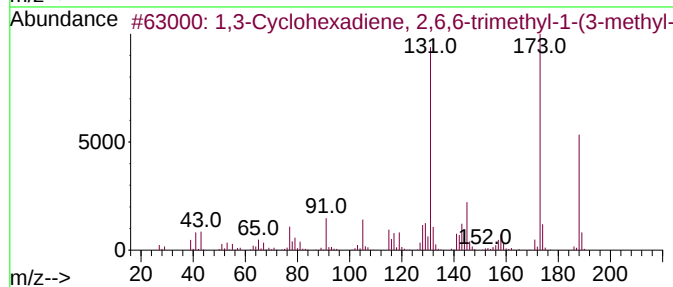
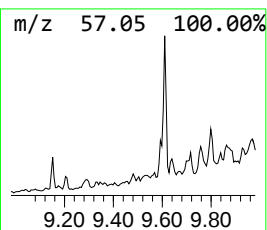
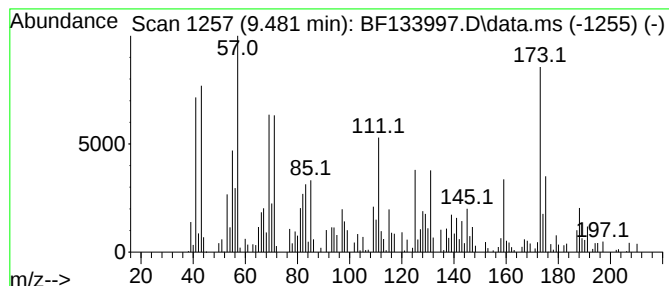
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.481 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.481	3.64 ng	105188	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclohexadiene, 2,6,6-trimet...	188	C14H20	052260-01-2	43		
2	1,1,5,6-Tetramethyl-1,2,3,4-tetr...	188	C14H20	031197-54-3	42		
3	1H-Inden-1-one, 2,3-dihydro-3,3,...	188	C13H16O	055255-42-0	42		
4	1-naphthalenol, 4-methoxy-3-methyl-	188	C12H12O2	1000400-16-9	38		
5	4'-(Trifluoromethyl)acetophenone	188	C9H7F3O	000709-63-7	30		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
Operator : CG\JU
Sample : 03398-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
WC-1

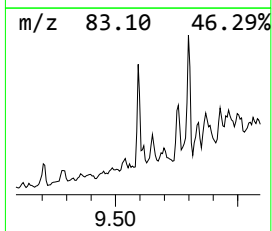
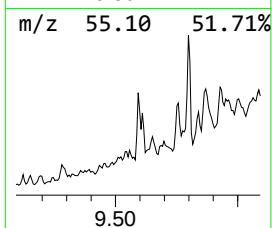
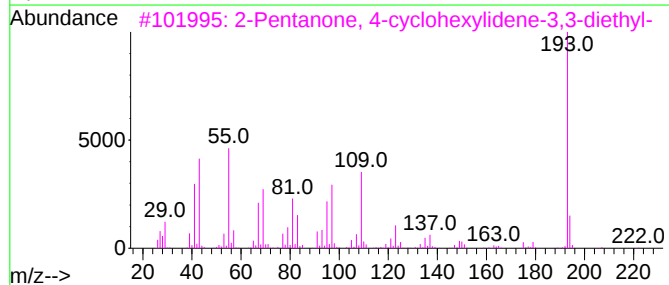
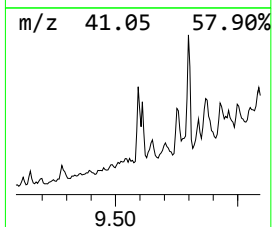
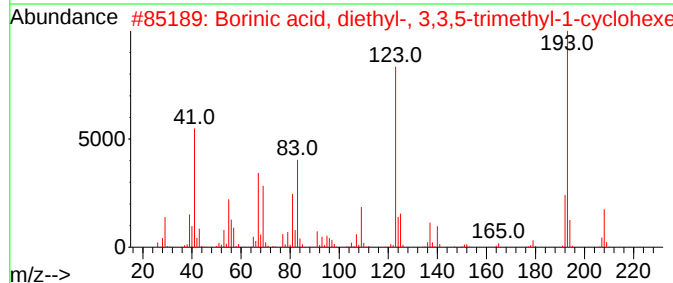
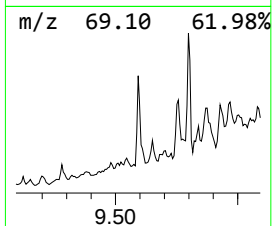
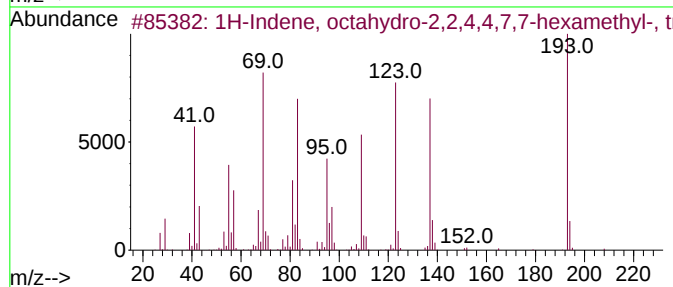
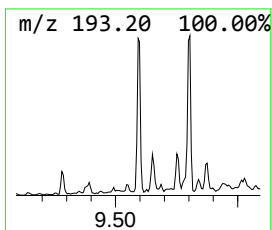
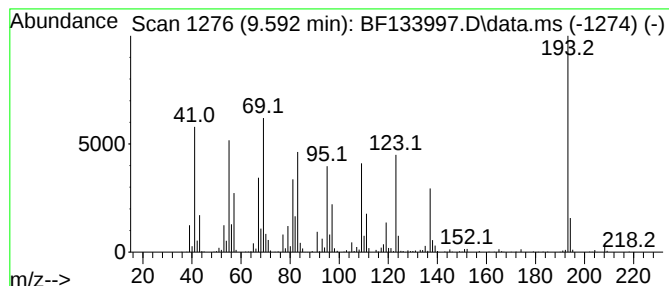
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.592 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	26.60 ng	768449	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	43
2			Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	38
3			2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	37
4			1-Methyl-3-(trifluoromethyl)-1H...	193	C7H10F3N3	1000511-73-1	35
5			1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Sample : 03398-01
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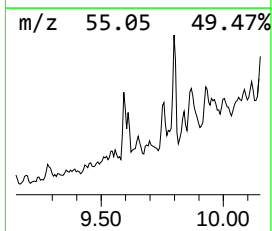
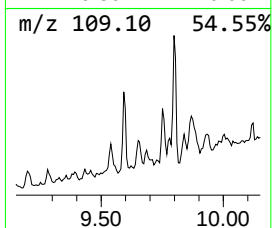
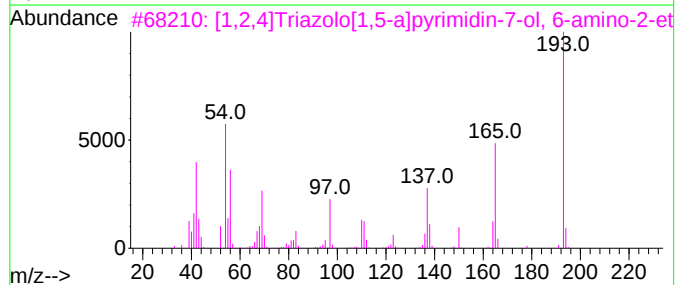
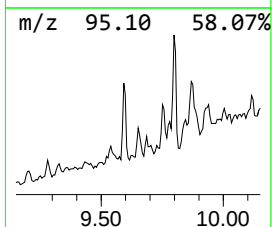
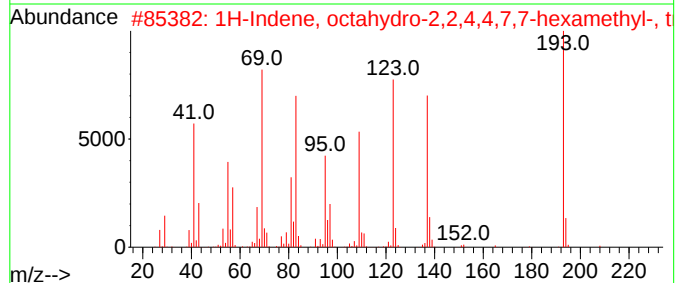
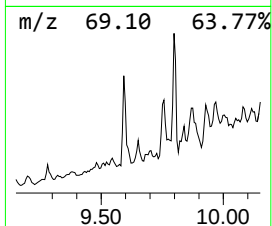
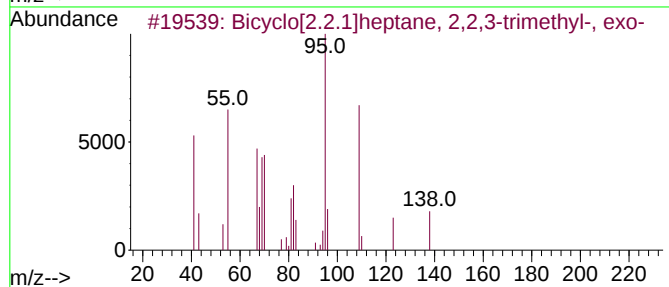
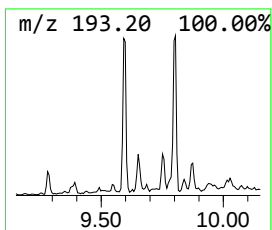
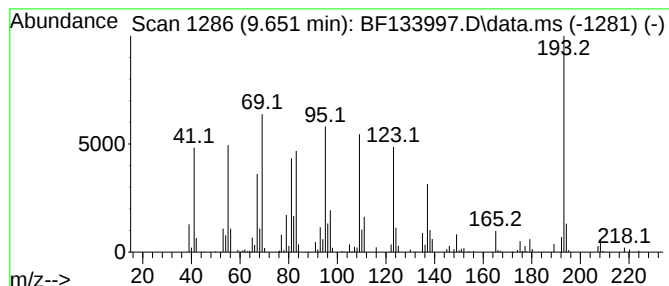
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Bicyclo[2.2.1]heptane, 2,2,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.651	10.89 ng	314723	Acenaphthene-d10		9.892	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptane, 2,2,3-tri...		138	C10H18	020536-41-8	60
2	1H-Indene, octahydro-2,2,4,4,7,7...		208	C15H28	054832-83-6	50
3	[1,2,4]Triazolo[1,5-a]pyrimidin...		193	C8H11N5O	1000351-50-1	38
4	Naphthalene, decahydro-1,6-dimet...		208	C15H28	029788-41-8	35
5	Pyrazolo[5,1-c]-as-triazine-3-ca...		193	C6H7N7O	016111-78-7	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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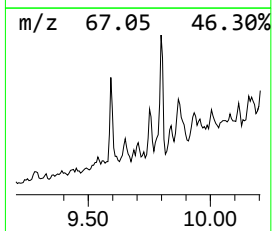
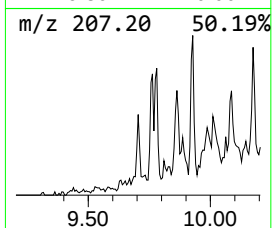
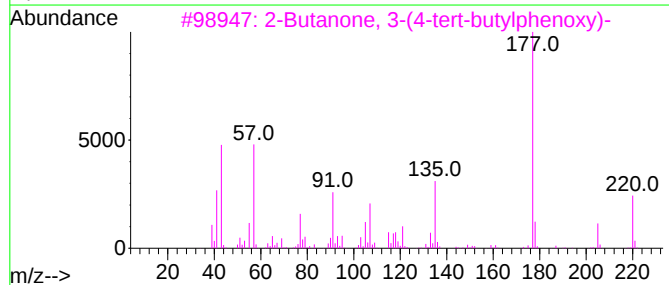
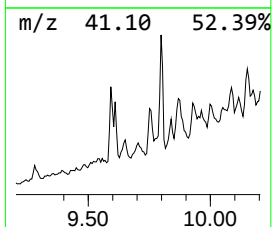
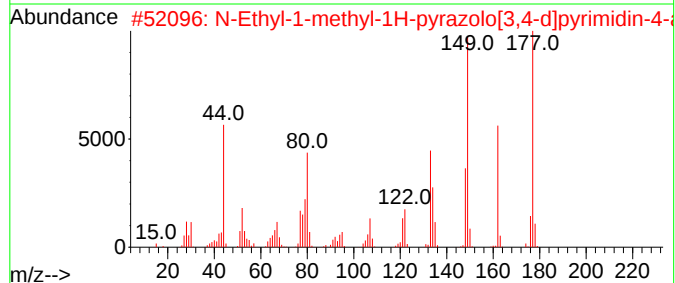
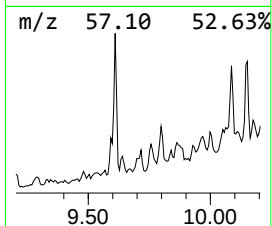
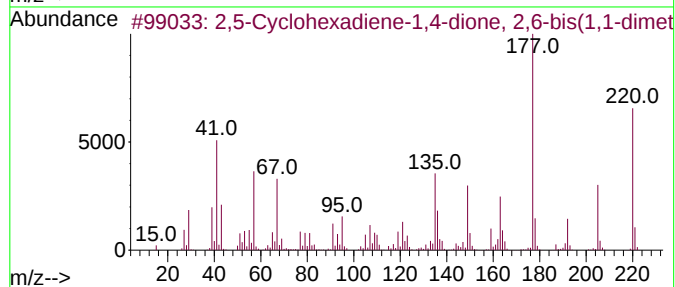
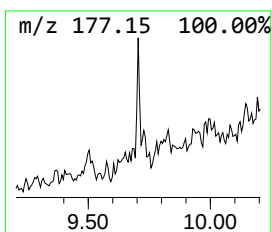
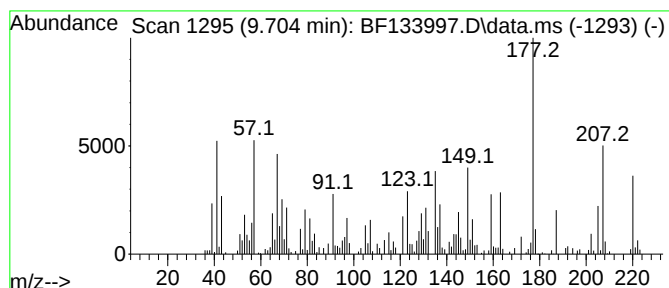
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.704	4.65 ng	134377	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	62		
2	N-Ethyl-1-methyl-1H-pyrazolo[3,4...	177	C8H11N5	005334-50-9	38		
3	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	38		
4	2-Acetyl-3,4,5,6-tetrafluorobenz...	220	C9H4F4O2	1000461-12-2	38		
5	Thiazole, 2-amino-4-(pyridin-3-yl)-	177	C8H7N3S	1000317-06-1	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Sample : 03398-01
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ALS Vial : 16 Sample Multiplier: 1

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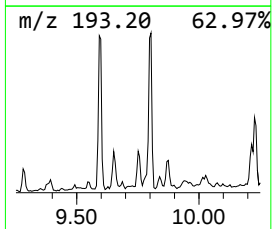
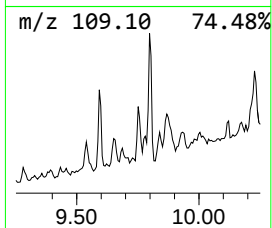
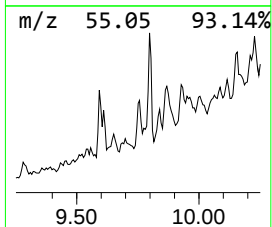
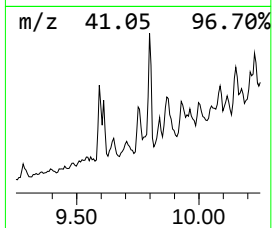
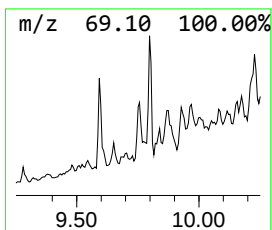
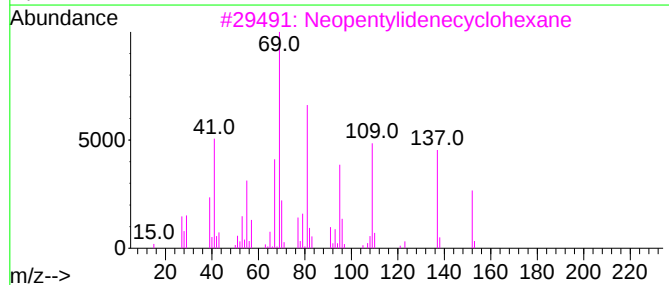
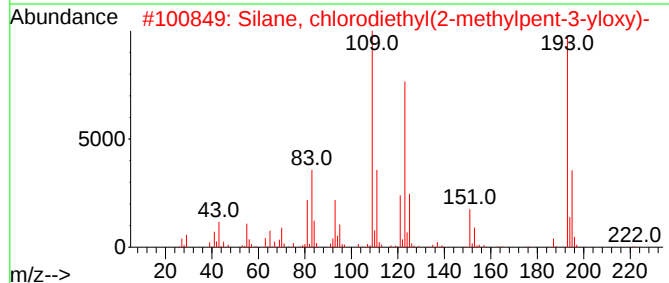
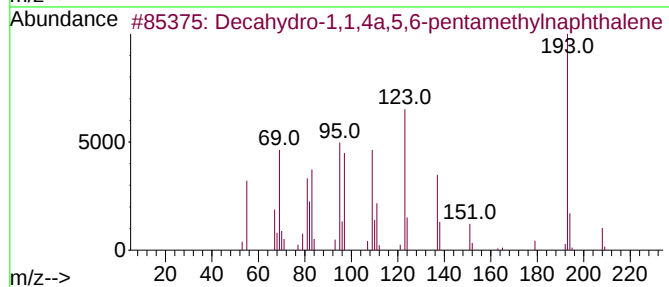
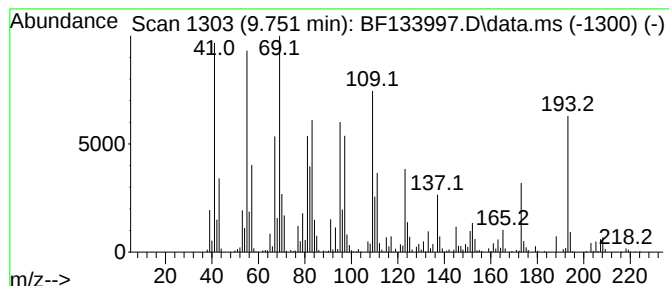
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.751 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.751	21.55 ng	622655	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	50
2			Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-79-1	46
3			Neopentylidenecyclohexane	152	C11H20	039546-80-0	43
4			1H-Pyrazole, 1-methyl-4-(4,4,5,5...	208	C10H17BN2O2	1000319-69-0	25
5			2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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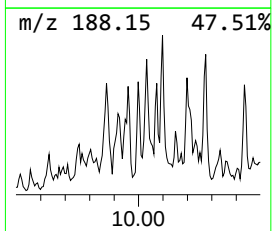
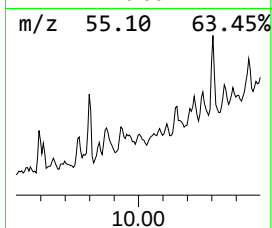
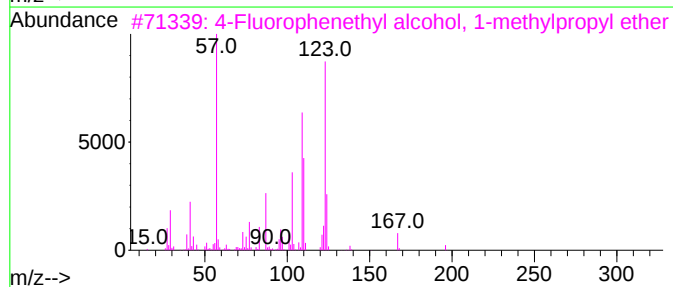
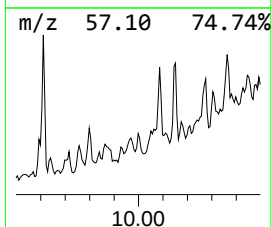
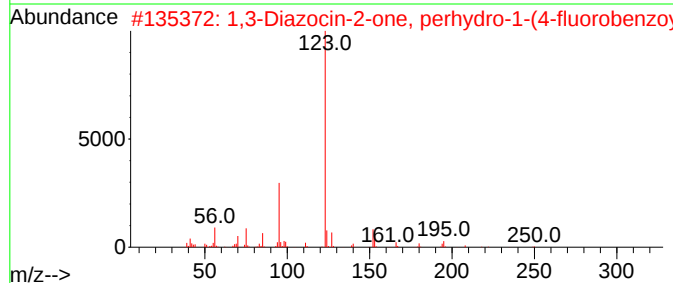
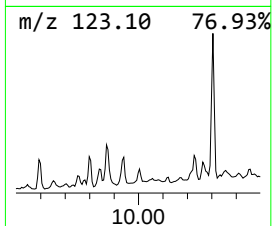
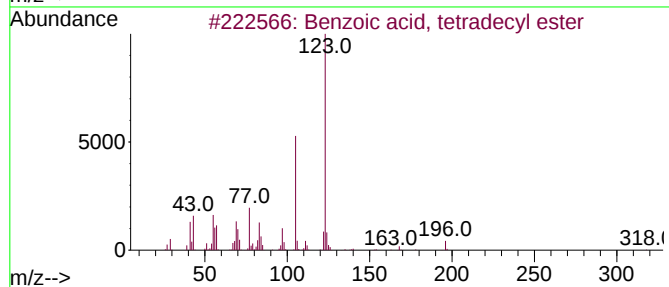
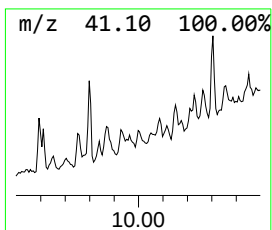
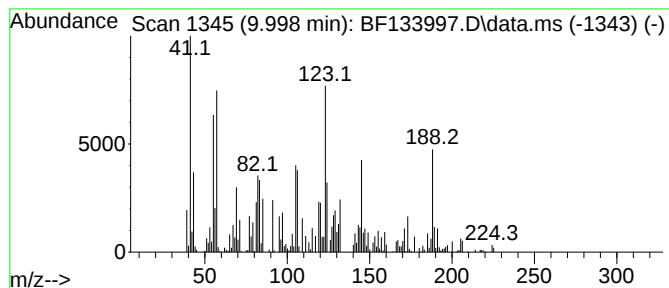
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown9.998 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	10.64 ng	307454	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, tetradecyl ester	318	C21H34O2	1000340-22-7	14
2			1,3-Diazocin-2-one, perhydro-1-(...	250	C13H15FN2O2	1000267-45-2	14
3			4-Fluorophenethyl alcohol, 1-met...	196	C12H17FO	1000394-95-0	14
4			4-Fluorobenzoic acid, 3-pentadec...	350	C22H35FO2	1000280-68-4	14
5			Bicyclo[2.1.1]hexane-5-carboxyli...	182	C10H14O3	1000217-20-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Misc :
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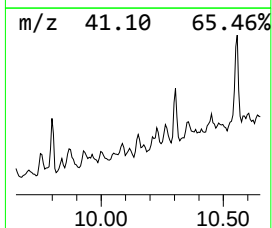
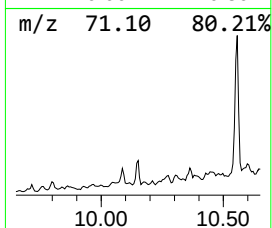
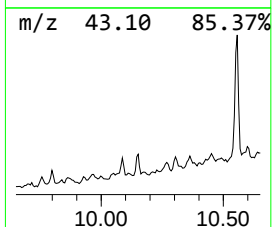
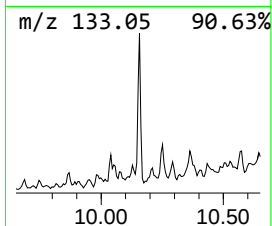
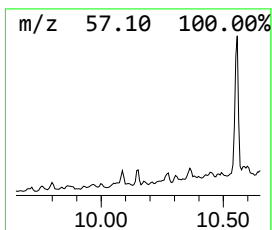
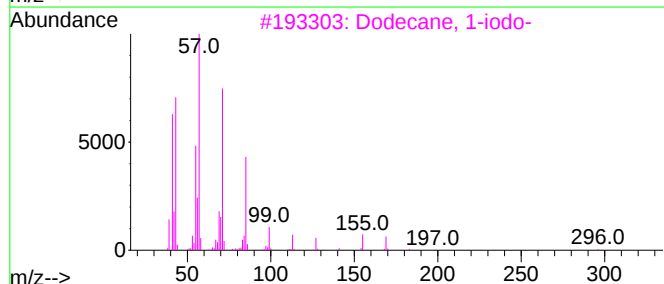
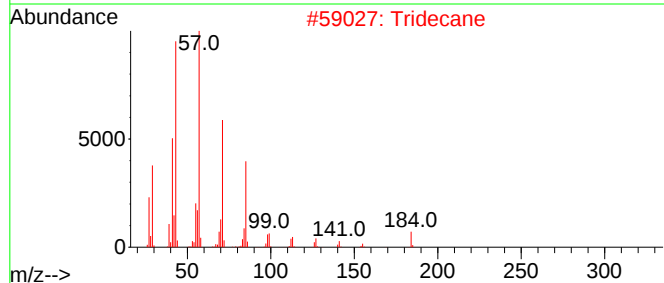
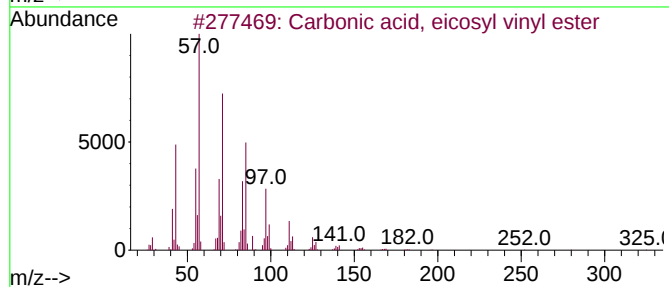
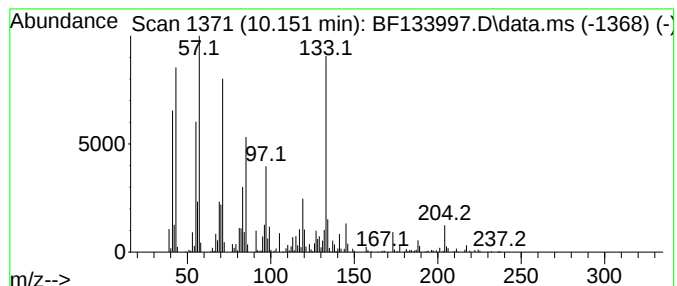
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown10.151 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.151	23.47 ng	678084	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	43
2			Tridecane	184	C13H28	000629-50-5	38
3			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	38
4			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	35
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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ALS Vial : 16 Sample Multiplier: 1

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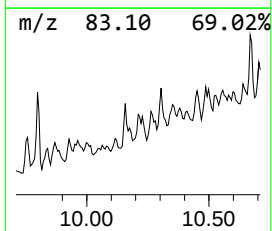
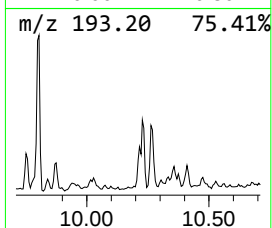
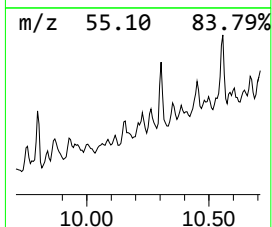
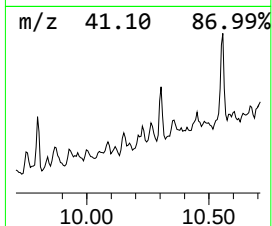
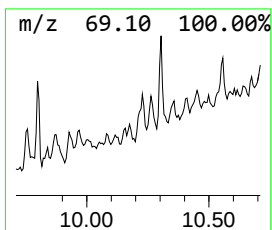
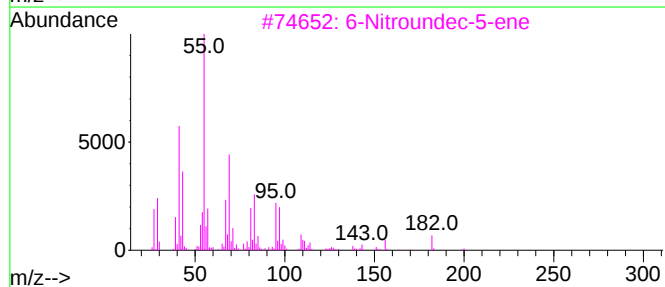
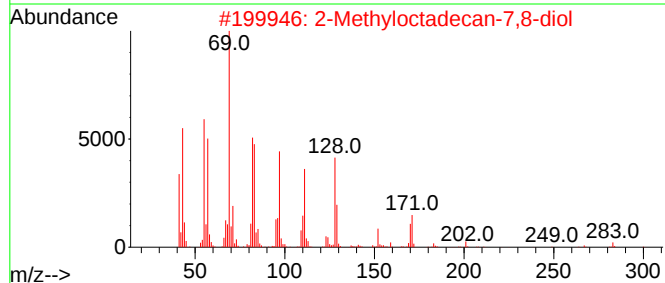
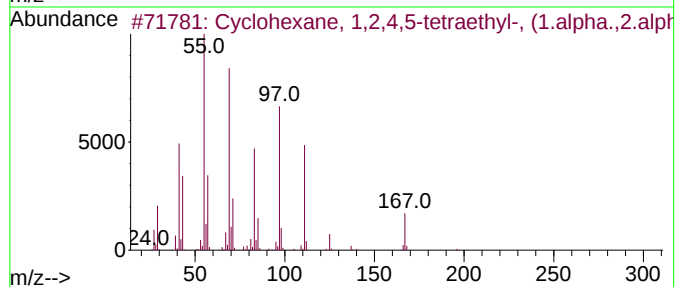
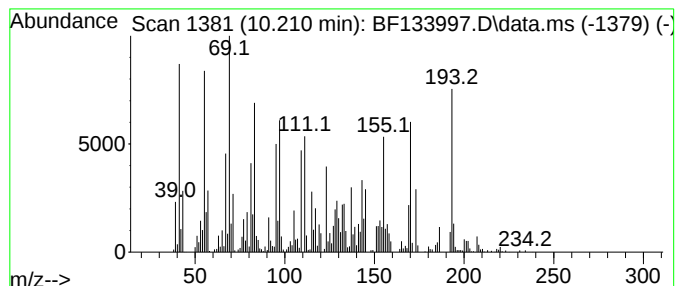
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.210 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.210	16.15 ng	466516	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,2,4,5-tetraethyl-...	196	C14H28	061142-24-3	38
2			2-Methyloctadecan-7,8-diol	300	C19H40O2	1000130-91-8	27
3			6-Nitroundec-5-ene	199	C11H21NO2	1000192-40-3	25
4			Crotyl methacrylate	140	C8H12O2	007376-45-6	25
5			1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
Operator : CG\JU
Sample : 03398-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

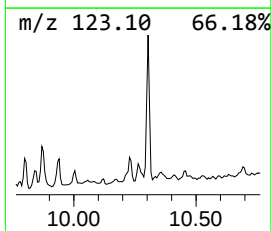
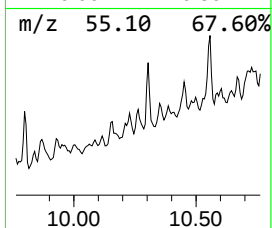
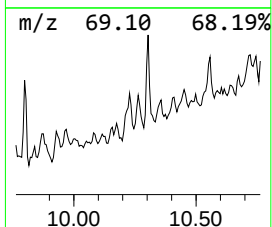
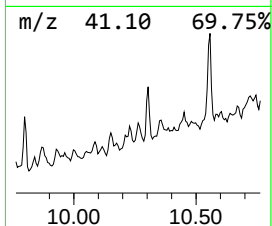
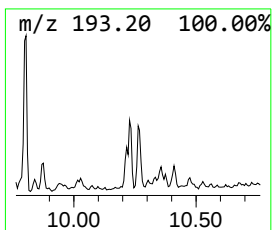
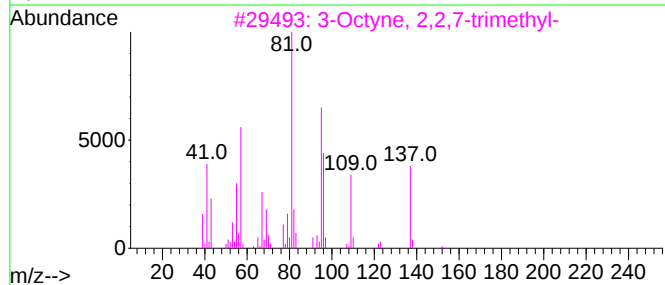
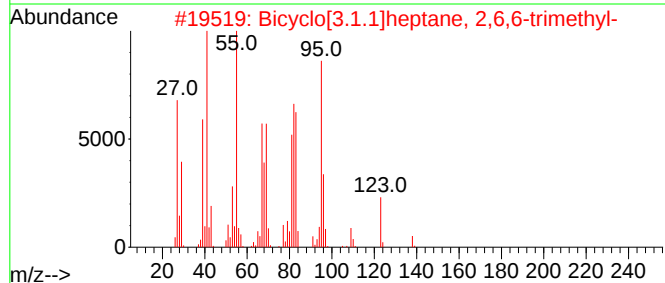
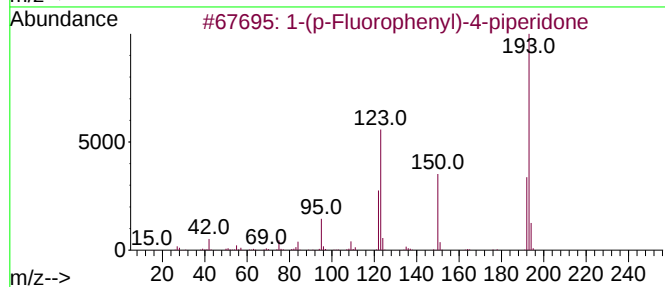
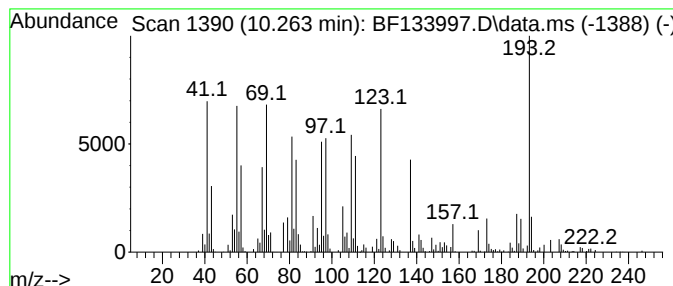
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown10.263 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.263	19.57 ng	565284	Acenaphthene-d10	9.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	25		
2	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	18		
3	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	11		
4	2-Nonen-4-yn-1-ol, (Z)-	138	C9H14O	134225-90-4	11		
5	Cyclohexane, 1-(cyclohexylmethyl)...	194	C14H26	054823-97-1	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
Operator : CG\JU
Sample : 03398-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

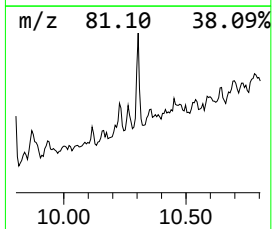
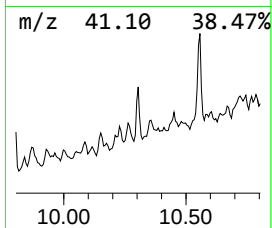
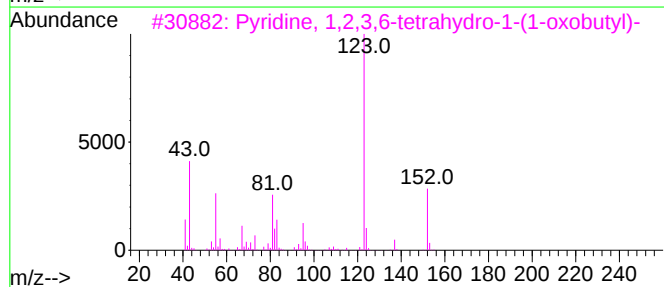
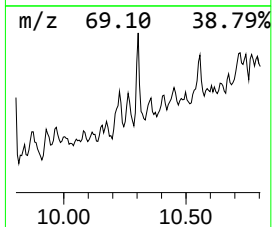
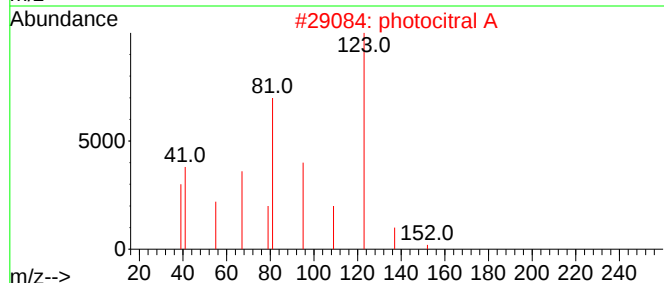
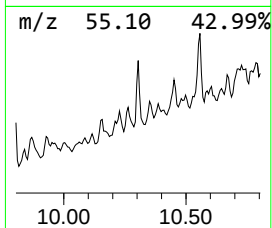
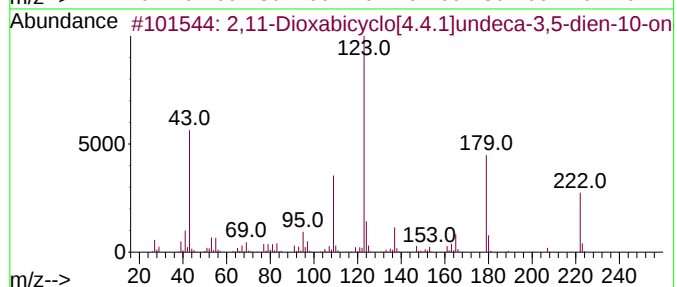
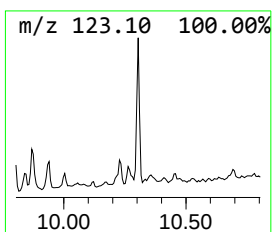
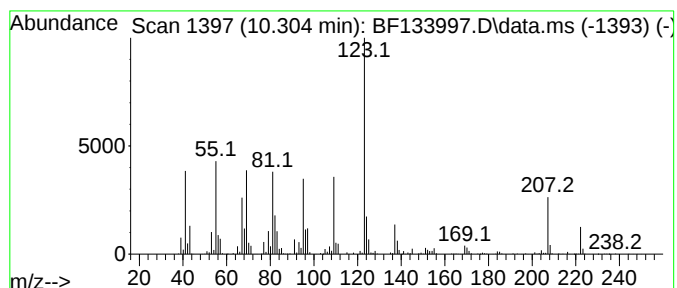
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,11-Dioxabicyclo[4.4.1]und... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.304	44.94 ng	1298330	Acenaphthene-d10		9.892	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,11-Dioxabicyclo[4.4.1]undeca-3...		222	C13H18O3	070412-52-1	59
2	photocitral A		152	C10H16O	055253-28-6	49
3	Pyridine, 1,2,3,6-tetrahydro-1-(...		153	C9H15NO	057150-46-6	47
4	2-Fluoro-N-(1,3-thiazol-2-yl)ben...		222	C10H7FN2OS	000319-38-0	47
5	3-Fluorobenzoic acid, 3-methylbu...		208	C12H13FO2	154559-38-3	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
Operator : CG\JU
Sample : 03398-01
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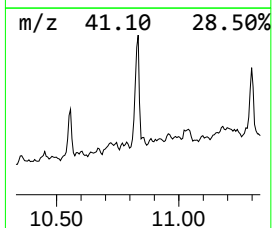
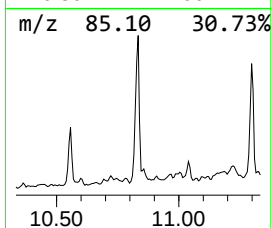
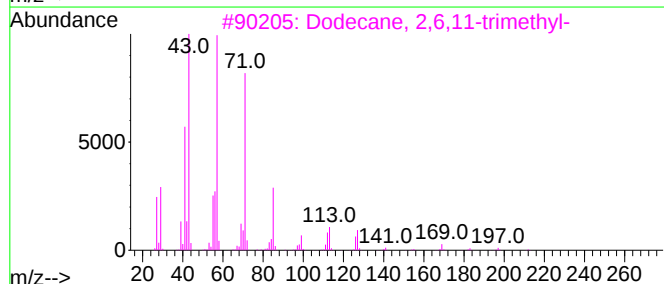
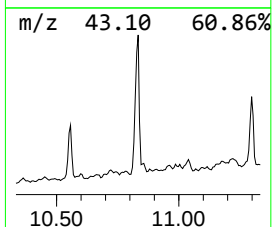
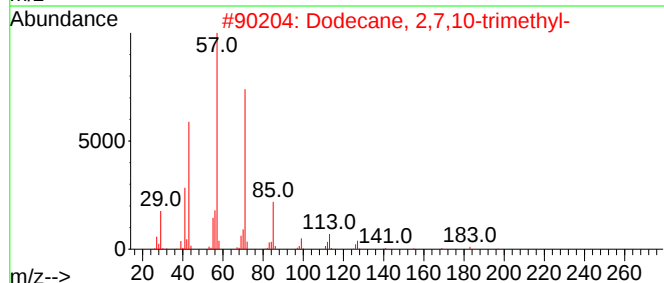
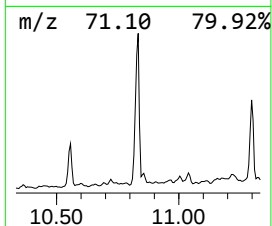
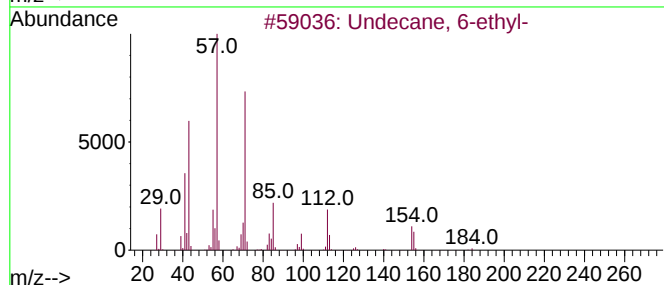
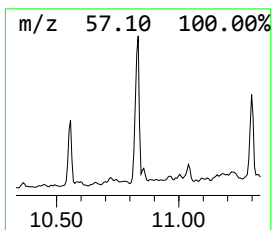
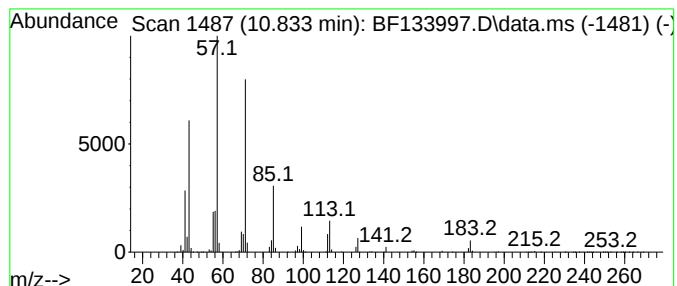
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Undecane, 6-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.834	41.33 ng	5822820	Phenanthrene-d10	11.398	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 6-ethyl-	184	C13H28	017312-60-6	83
2	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	72
3	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	72
4	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	64
5	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
Operator : CG\JU
Sample : 03398-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

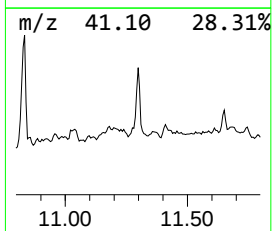
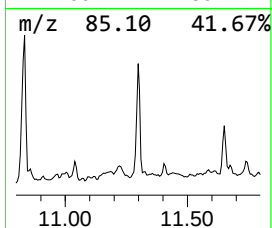
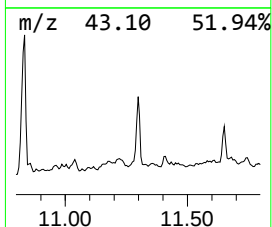
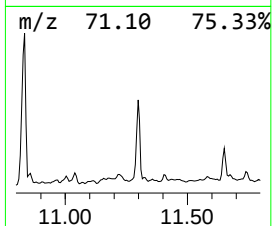
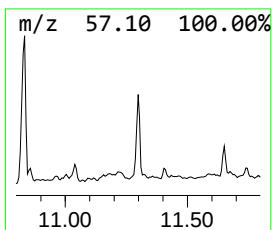
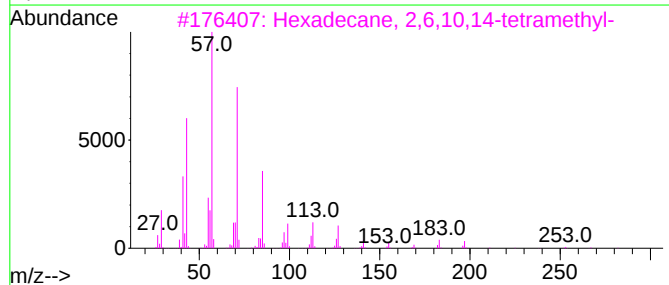
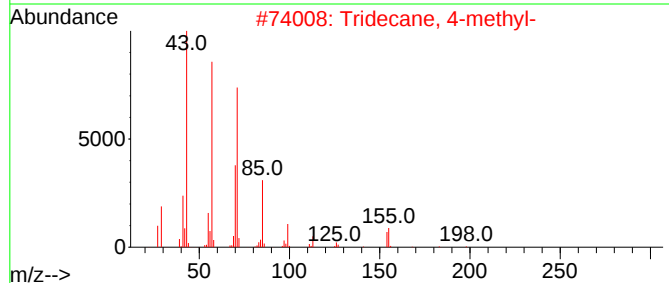
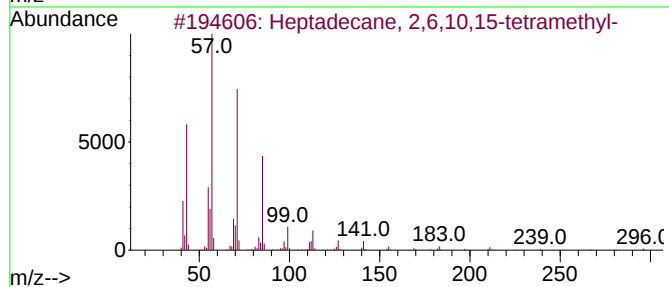
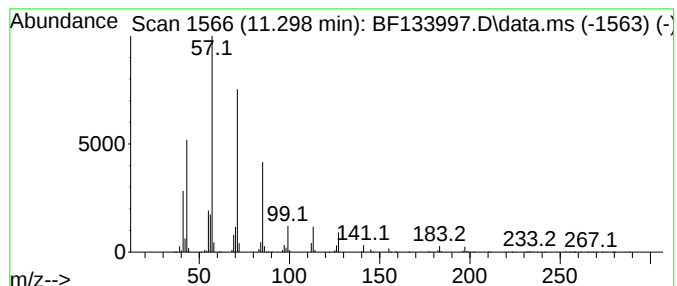
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Heptadecane, 2,6,10,15-tetr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	20.00 ng	2818010	Phenanthrene-d10	11.398

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2		Tridecane, 4-methyl-	198	C14H30	026730-12-1	87
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86
4		Tridecane, 2-methyl-	198	C14H30	001560-96-9	83
5		Dodecane, 4-methyl-	184	C13H28	006117-97-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
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Acq On : 27 Jun 2023 18:28
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Misc :
ALS Vial : 16 Sample Multiplier: 1

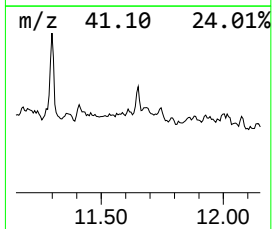
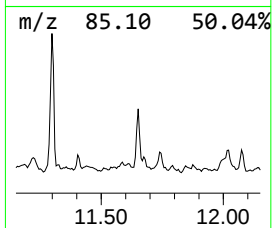
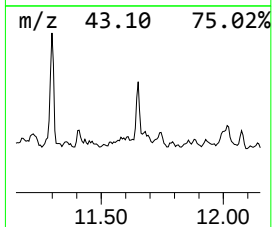
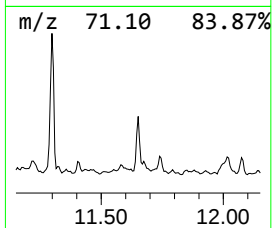
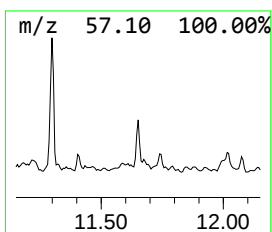
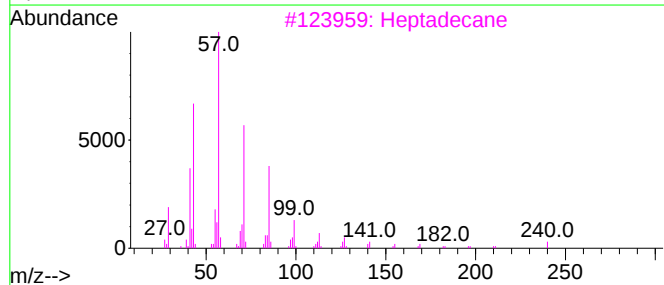
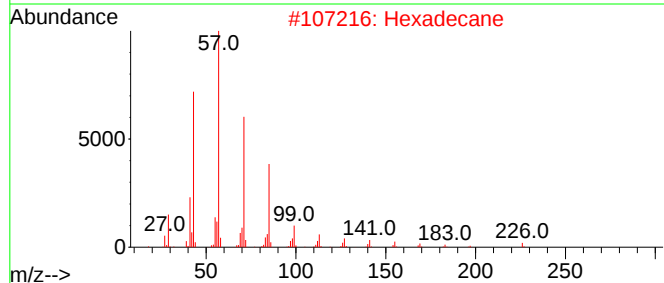
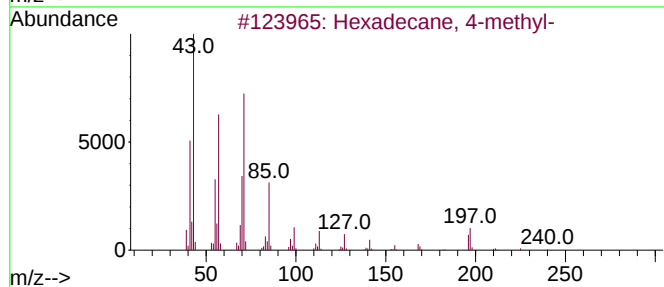
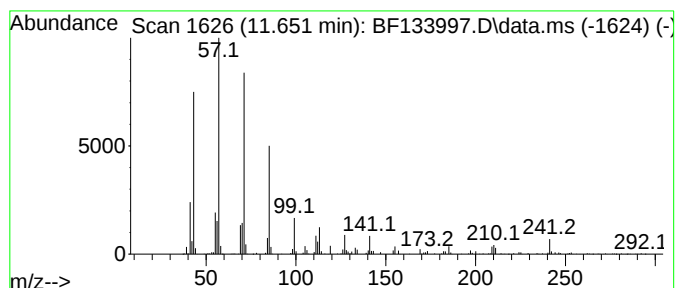
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Hexadecane, 4-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.651	5.92 ng	833453	Phenanthrene-d10	11.398	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 4-methyl-	240	C17H36	025117-26-4	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
5	Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
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Sample : 03398-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

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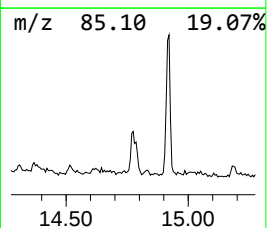
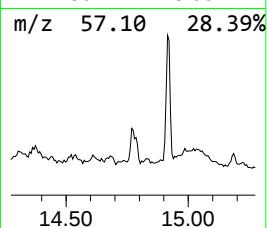
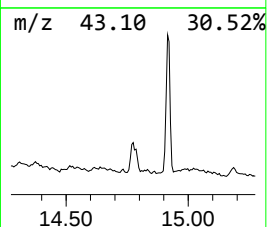
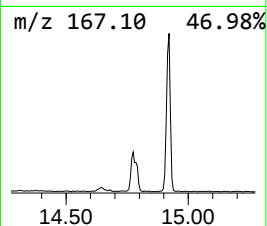
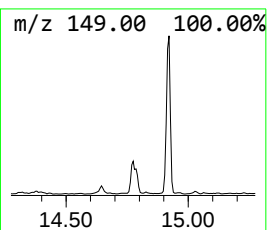
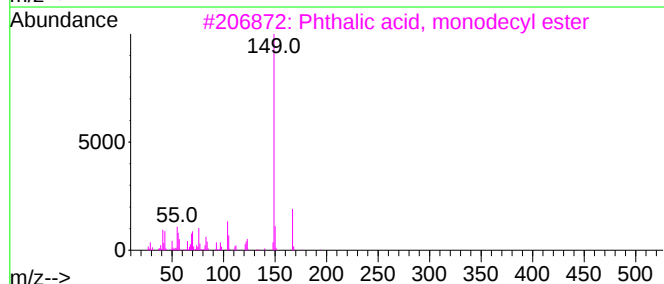
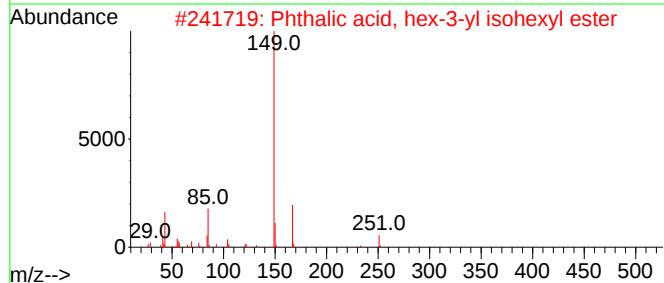
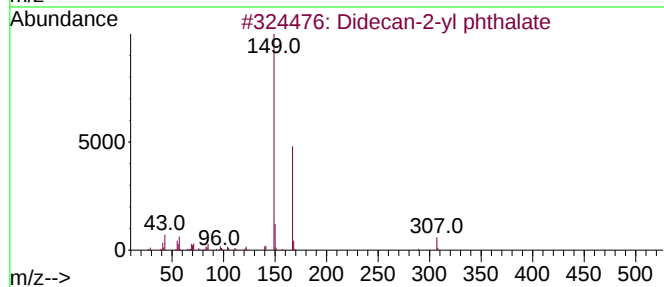
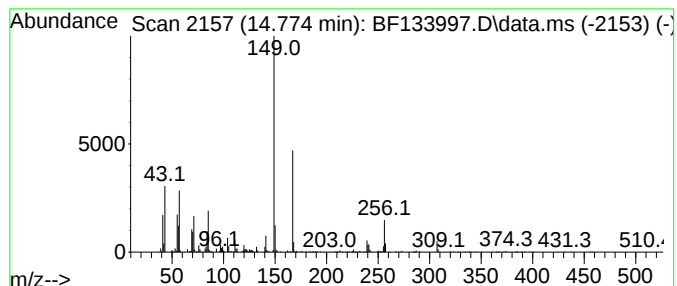
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Didecan-2-yl phthalate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.774	39.89 ng	716840	Chrysene-d12	14.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Didecan-2-yl phthalate	446	C28H46O4	028029-89-2	59
2			Phthalic acid, hex-3-yl isohexyl...	334	C20H30O4	1000356-95-6	58
3			Phthalic acid, monodecyl ester	306	C18H26O4	024539-60-4	53
4			6H-Thieno[2,3-b]pyrrole-5-carbox...	167	C7H5N02S	051856-25-8	53
5			Phthalic acid, hexyl 4-methylpen...	334	C20H30O4	1000356-87-6	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
Operator : CG\JU
Sample : 03398-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

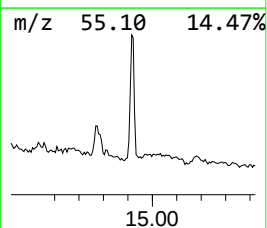
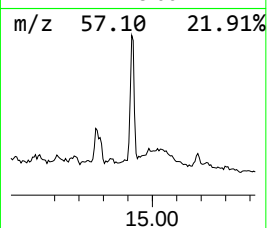
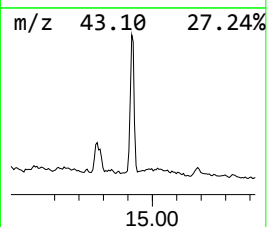
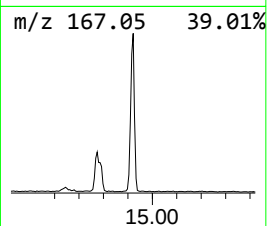
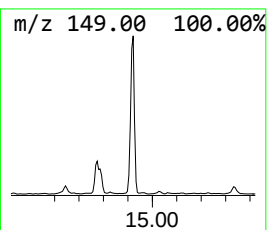
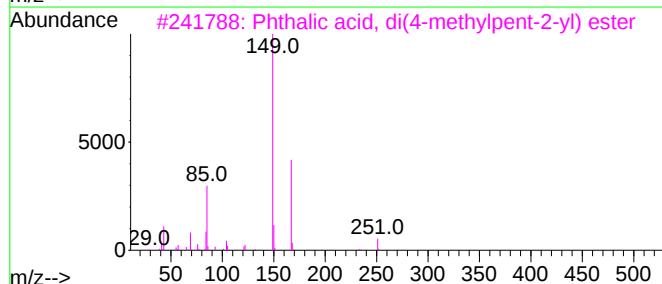
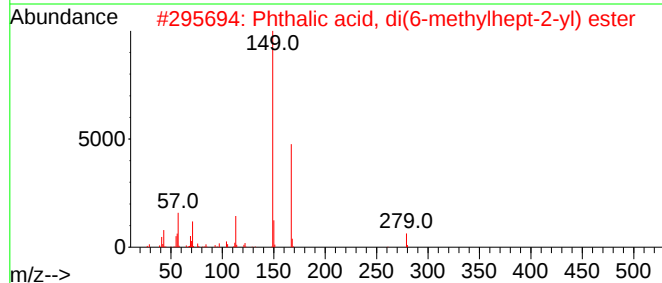
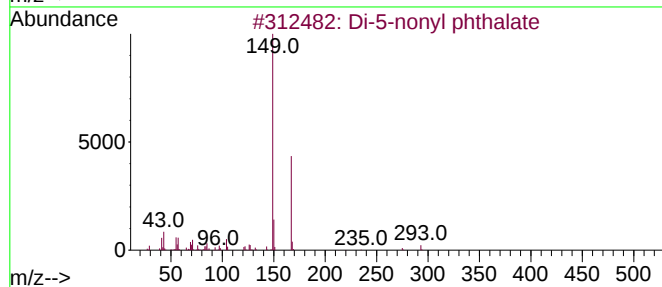
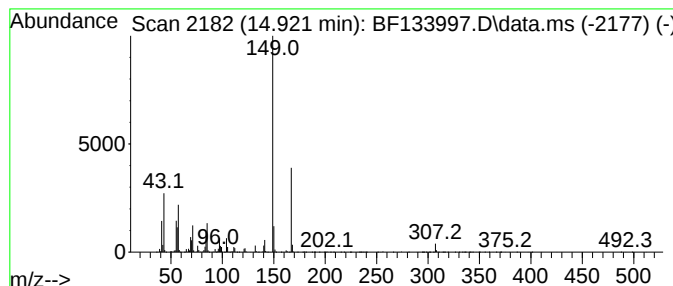
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Di-5-nonyl phthalate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.921	123.64 ng	1916520	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-5-nonyl phthalate	418	C26H42O4	094054-23-6	72
2			Phthalic acid, di(6-methylhept-2-yl) ester	390	C24H38O4	1000377-97-3	72
3			Phthalic acid, di(4-methylpent-2-yl) ester	334	C20H30O4	1010356-88-6	72
4			Di-2-nonyl phthalate	418	C26H42O4	059431-96-8	64
5			Phthalic acid, cyclohexylmethyl ...	332	C20H28O4	1000315-55-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062723\
Data File : BF133997.D
Acq On : 27 Jun 2023 18:28
Operator : CG\JU
Sample : 03398-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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
Butane, 2-metho...	2.152	51.4	ng	1471170	1	6.851	572137	20.0
2-Pentanone, 4-...	5.093	2.8	ng	78614	1	6.851	572137	20.0
Hexadecane, 2,6...	9.151	3.4	ng	97894	3	9.892	577746	20.0
Decahydro-1,1,4...	9.281	7.1	ng	205710	3	9.892	577746	20.0
unknown9.481	9.481	3.6	ng	105188	3	9.892	577746	20.0
unknown9.592	9.592	26.6	ng	768449	3	9.892	577746	20.0
Bicyclo[2.2.1]h...	9.651	10.9	ng	314723	3	9.892	577746	20.0
2,5-Cyclohexadi...	9.704	4.7	ng	134377	3	9.892	577746	20.0
unknown9.751	9.751	21.6	ng	622655	3	9.892	577746	20.0
unknown9.998	9.998	10.6	ng	307454	3	9.892	577746	20.0
unknown10.151	10.151	23.5	ng	678084	3	9.892	577746	20.0
unknown10.210	10.210	16.1	ng	466516	3	9.892	577746	20.0
unknown10.263	10.263	19.6	ng	565284	3	9.892	577746	20.0
2,11-Dioxabicyc...	10.304	44.9	ng	1298330	3	9.892	577746	20.0
Undecane, 6-ethyl-	10.834	41.3	ng	5822820	4	11.398	2818010	20.0
Heptadecane, 2,...	11.298	20.0	ng	2818010	4	11.398	2818010	20.0
Hexadecane, 4-m...	11.651	5.9	ng	833453	4	11.398	2818010	20.0
Didecan-2-yl ph...	14.774	39.9	ng	716840	5	14.051	359404	20.0
Di-5-nonyl phth...	14.921	123.6	ng	1916520	6	15.551	310014	20.0