

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
 Data File : BF141039.D
 Acq On : 30 Dec 2024 18:58
 Operator : RC/JU
 Sample : P5386-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MOO-24-00398

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-BF122624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141039.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.875	294	303	310	rBV	1326726	2172612	2.64%	0.385%
2	4.410	386	394	400	rBV	3414905	5347105	6.49%	0.947%
3	5.169	488	523	529	rBV	12220879	82353185	100.00%	14.585%
4	5.428	561	567	569	rBV	2879528	4365680	5.30%	0.773%
5	5.451	569	571	587	rVB	3298996	4253015	5.16%	0.753%
6	5.687	605	611	616	rBV	6779084	9195304	11.17%	1.629%
7	6.004	655	665	674	rBV	2273683	3176919	3.86%	0.563%
8	6.298	705	715	720	rBV	7608197	12441404	15.11%	2.203%
9	6.375	720	728	731	rVV	14330533	29089637	35.32%	5.152%
10	6.404	731	733	736	rVV	10585260	12343291	14.99%	2.186%
11	6.445	736	740	745	rVV	10960972	17672967	21.46%	3.130%
12	6.481	745	746	749	rVV2	1263648	1506819	1.83%	0.267%
13	6.528	749	754	759	rVV	10174889	15439625	18.75%	2.734%
14	6.586	759	764	771	rVB2	1349273	2140529	2.60%	0.379%
15	6.681	771	780	790	rVB	16734812	39325686	47.75%	6.965%
16	6.792	791	799	802	rBV2	4096508	7117949	8.64%	1.261%
17	6.845	802	808	811	rVV2	12055972	20524195	24.92%	3.635%
18	6.875	811	813	814	rVV	3621475	3556146	4.32%	0.630%
19	6.910	814	819	824	rVV2	12346727	27023540	32.81%	4.786%
20	6.957	824	827	830	rVV	4480328	5789345	7.03%	1.025%
21	7.004	830	835	844	rVB2	11645680	21581975	26.21%	3.822%
22	7.086	844	849	851	rBV	6821130	8994090	10.92%	1.593%
23	7.116	851	854	857	rVV	6147889	7388750	8.97%	1.309%
24	7.163	857	862	869	rVB3	10766537	18493391	22.46%	3.275%
25	7.228	869	873	878	rBV	2766439	3611526	4.39%	0.640%
26	7.298	878	885	888	rBV	3211490	5105886	6.20%	0.904%
27	7.322	888	889	893	rVB	2097875	1766859	2.15%	0.313%
28	7.381	893	899	905	rBV3	8750875	15225856	18.49%	2.697%
29	7.433	905	908	911	rVB	1277904	1577919	1.92%	0.279%
30	7.481	911	916	919	rBV3	911223	1270799	1.54%	0.225%
31	7.522	919	923	925	rBV2	698119	1012071	1.23%	0.179%
32	7.645	933	944	952	rBV6	4758305	13729558	16.67%	2.432%
33	7.763	954	964	969	rBV4	12536333	45635090	55.41%	8.082%
34	7.881	981	984	988	rVB3	4954926	7142088	8.67%	1.265%
35	8.004	1000	1005	1008	rBV3	3470840	7281857	8.84%	1.290%
36	8.433	1074	1078	1082	rVB4	5233495	8068606	9.80%	1.429%

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Instrument :
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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-BF122624.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.510	1088	1091	1095	rVV3	3365511	4525635	5.50%	0.802%
38	8.551	1095	1098	1109	rVB	7816728	16806892	20.41%	2.977%
39	8.728	1122	1128	1132	rBV2	8806995	15472034	18.79%	2.740%
40	8.904	1155	1158	1163	rBV5	1376379	2116857	2.57%	0.375%
41	8.998	1171	1174	1178	rBV4	2363047	4424157	5.37%	0.784%
42	9.080	1184	1188	1191	rVB	2872243	3582881	4.35%	0.635%
43	9.116	1191	1194	1196	rBV	2403642	2870555	3.49%	0.508%
44	9.192	1203	1207	1211	rVB2	3034910	4083047	4.96%	0.723%
45	9.280	1217	1222	1227	rBV	7688301	12446781	15.11%	2.204%
46	9.510	1258	1261	1263	rBV4	1867676	2431542	2.95%	0.431%
47	9.586	1271	1274	1279	rBV4	3616089	6674005	8.10%	1.182%
48	9.745	1298	1301	1304	rBV3	2299411	3527014	4.28%	0.625%
49	9.792	1306	1309	1312	rVV	2884924	3827387	4.65%	0.678%
50	9.863	1318	1321	1327	rVB5	2586417	4199239	5.10%	0.744%
51	15.939	2351	2354	2359	rVB	1000350	1548444	1.88%	0.274%
52	17.939	2687	2694	2714	rVB	1108013	3384751	4.11%	0.599%

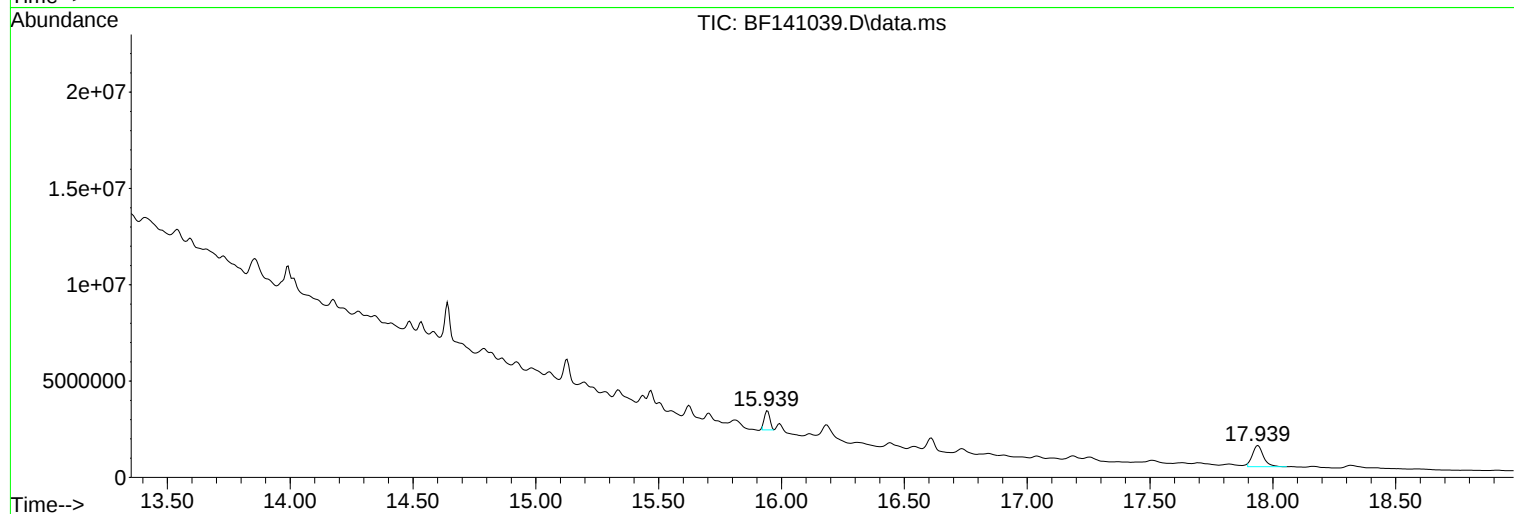
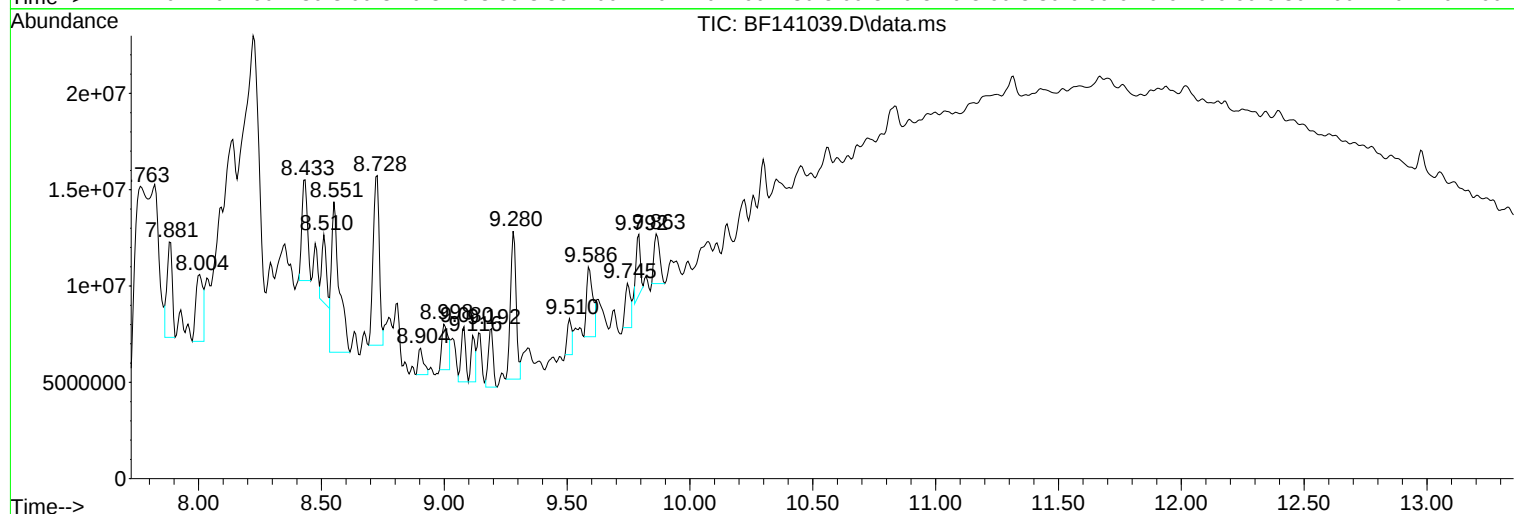
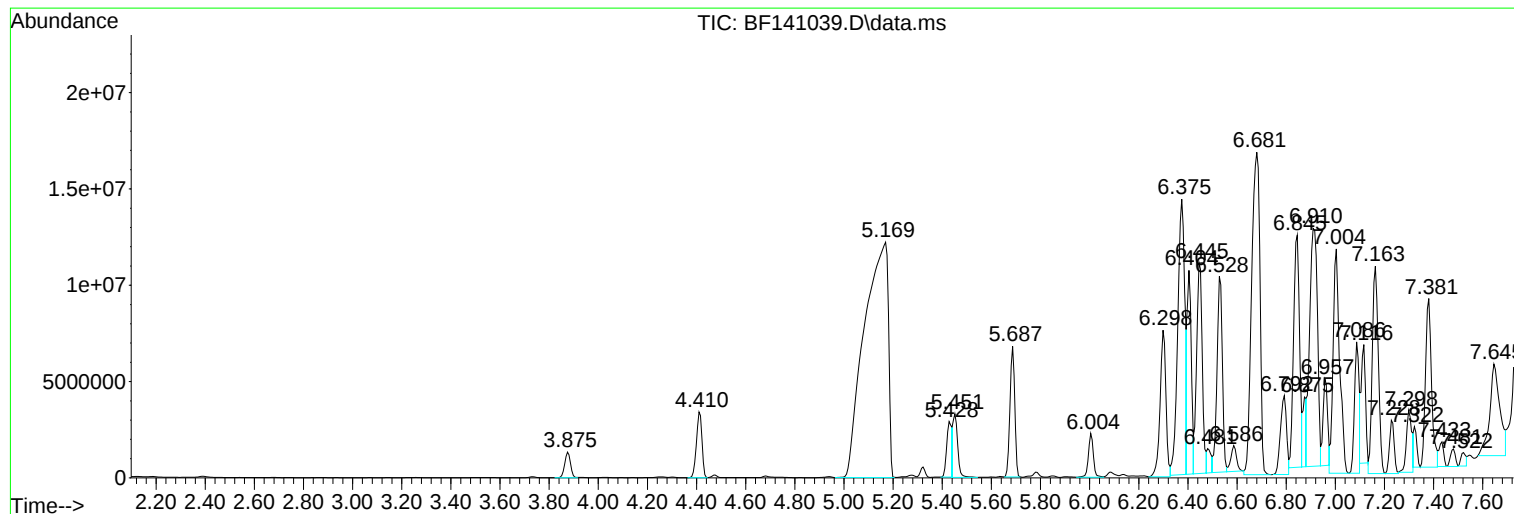
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

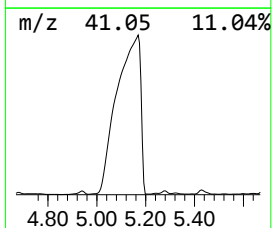
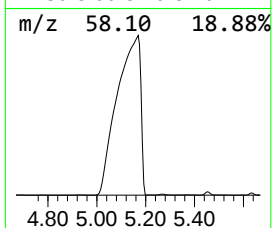
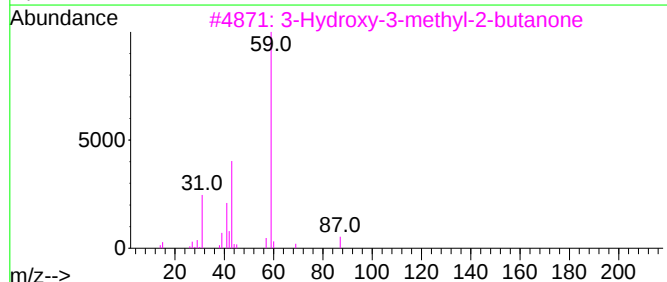
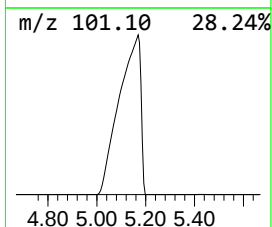
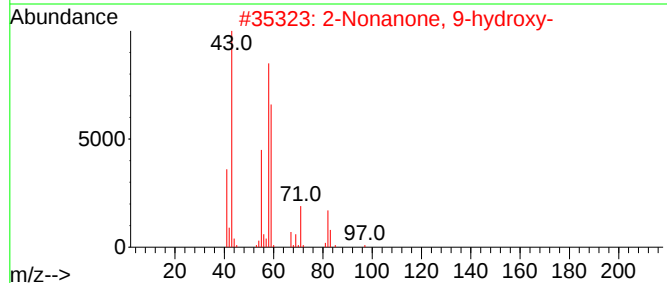
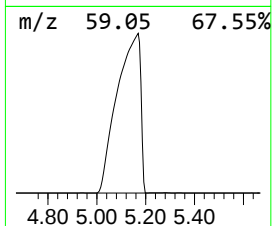
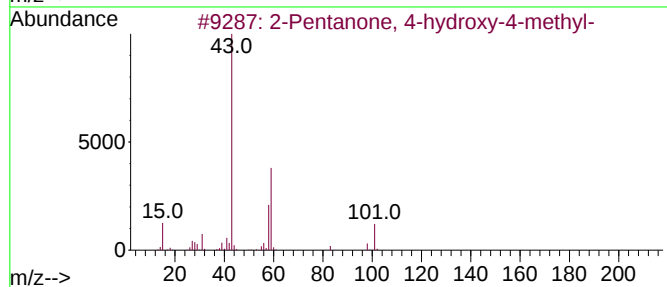
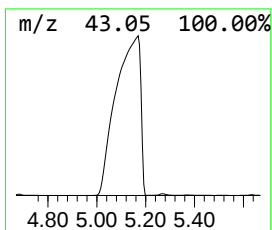
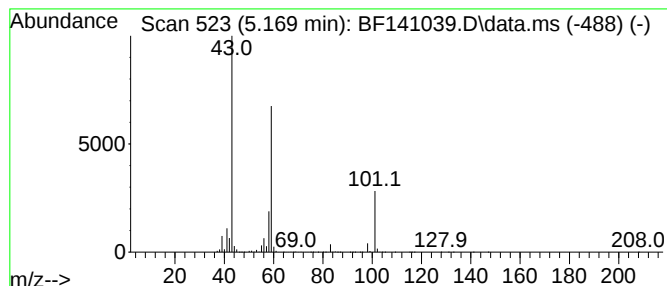
Instrument :
BNA_F
ClientSampleId :
MOO-24-00398

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.169	80.25 ng	82353200	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	42
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Acetone	58	C3H6O	000067-64-1	10



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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-24-00398

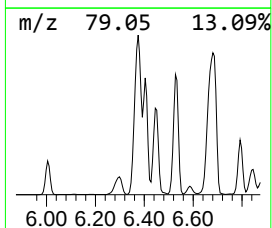
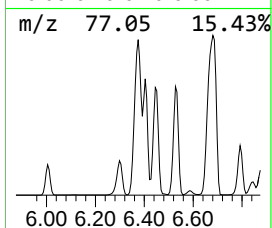
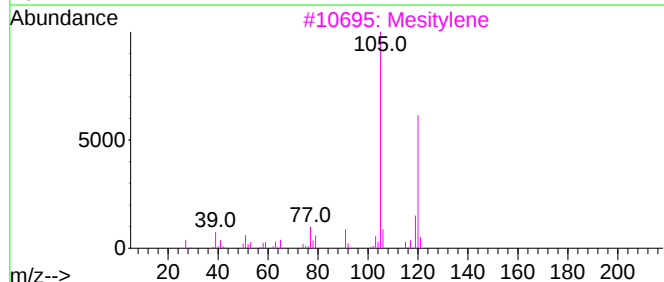
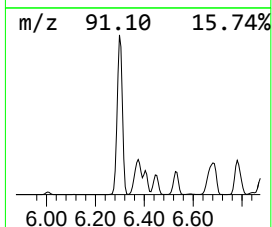
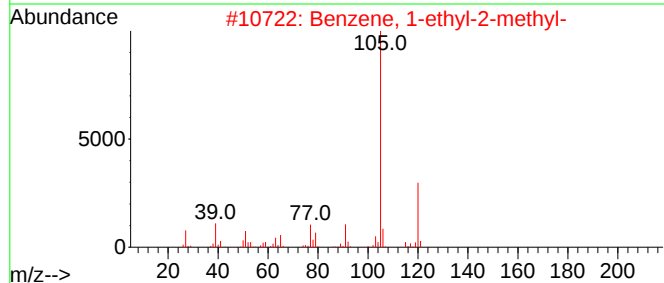
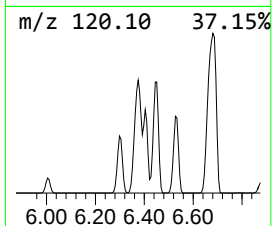
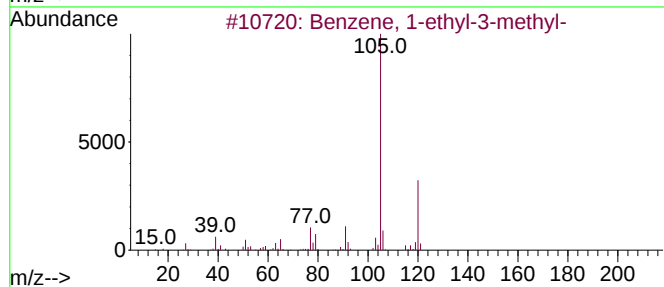
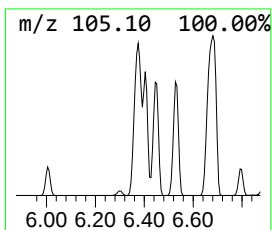
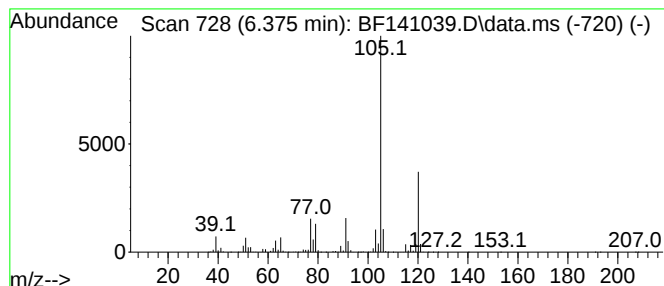
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.375	28.35 ng	29089600	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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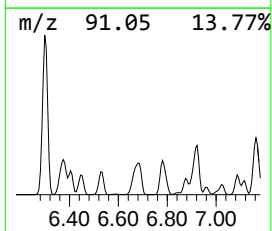
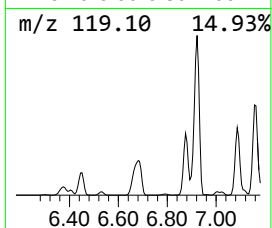
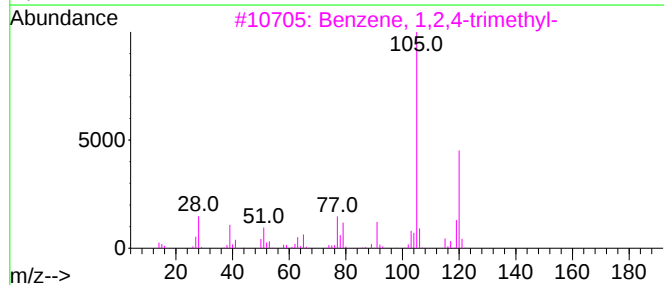
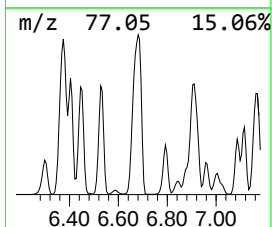
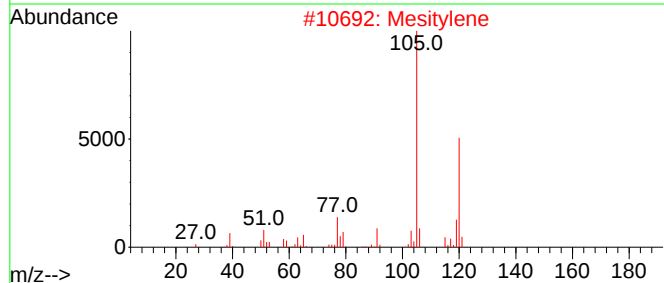
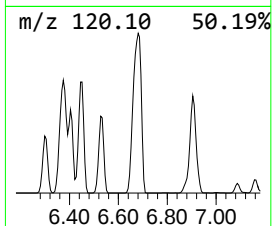
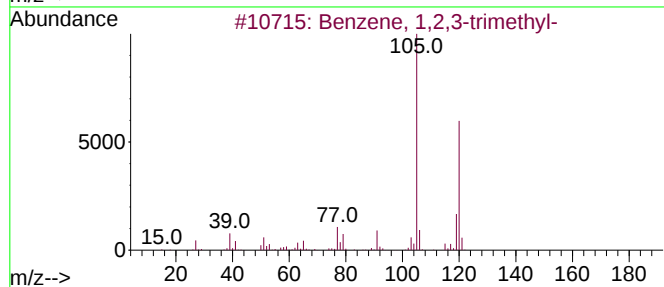
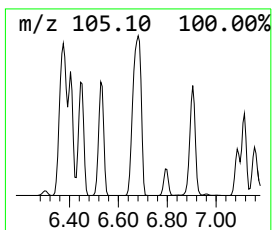
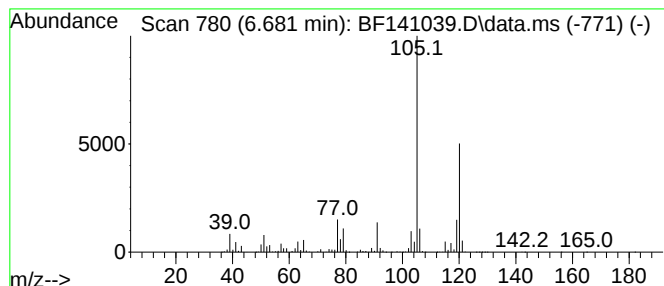
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.681	38.32 ng	39325700	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	97
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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Misc :
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ClientSampleId :
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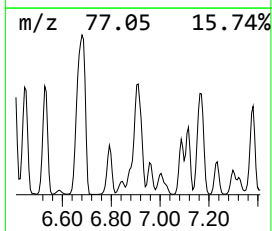
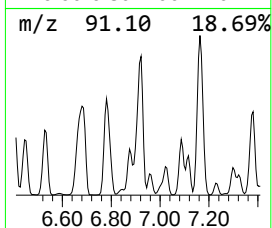
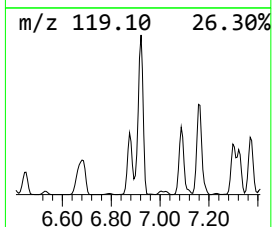
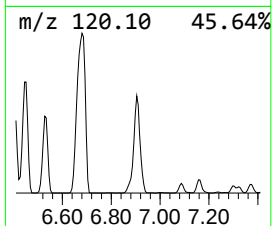
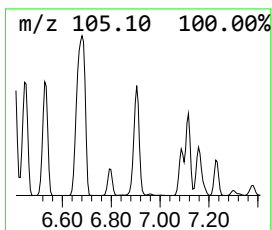
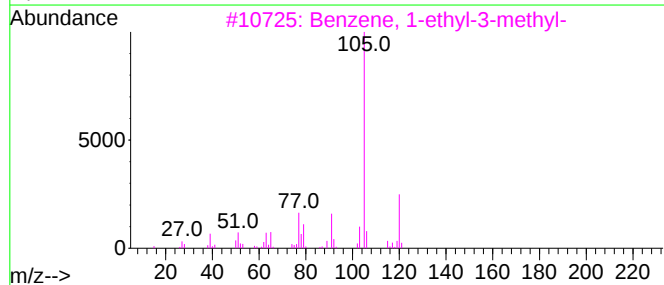
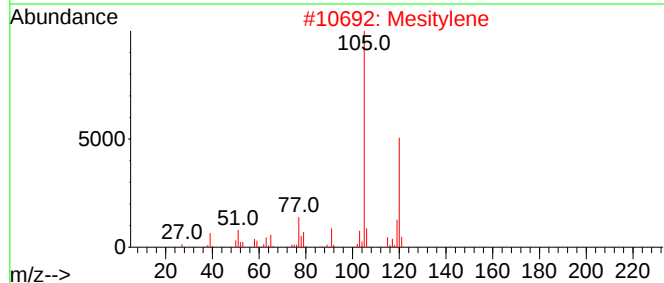
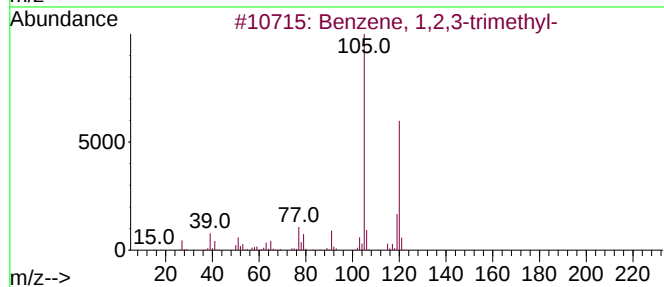
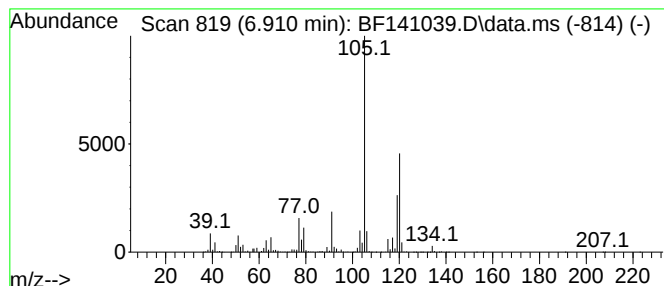
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Mesitylene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.910	26.33 ng	27023500	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
2			Mesitylene	120	C9H12	000108-67-8	87
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	87
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	87
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	87



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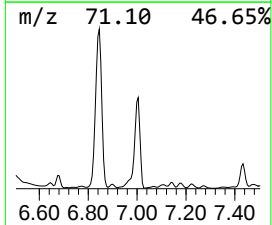
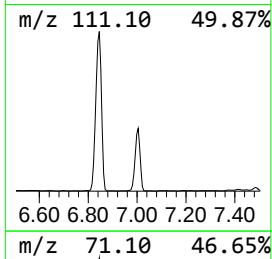
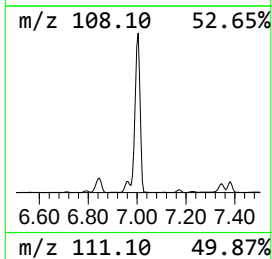
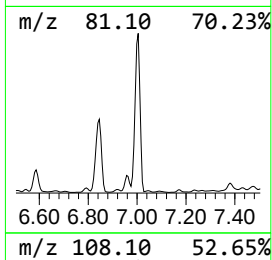
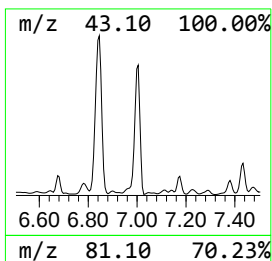
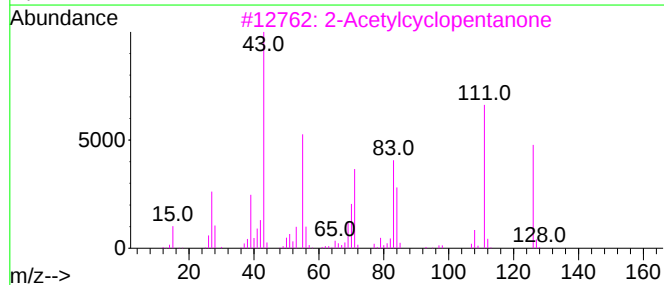
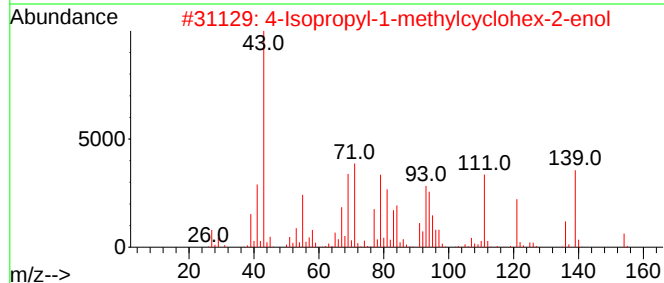
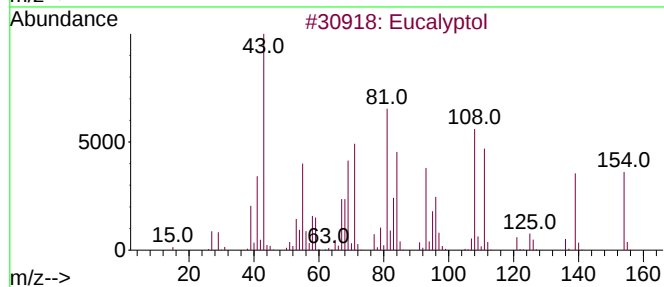
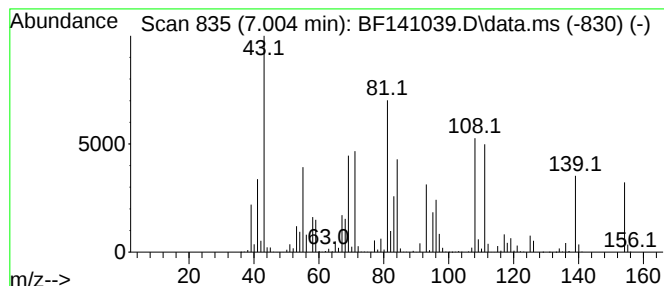
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Eucalyptol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.004	21.03 ng	21582000	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	95
2			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	37
3			2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	25
4			2-Acetyl cyclohexanone	154	C9H14O2	006126-53-0	22
5			2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-24-00398

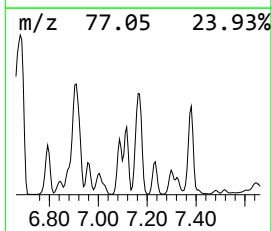
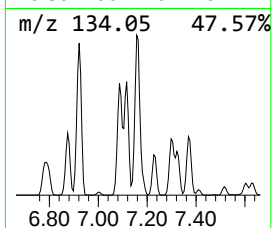
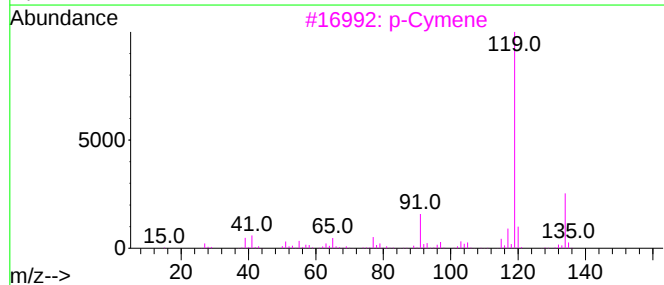
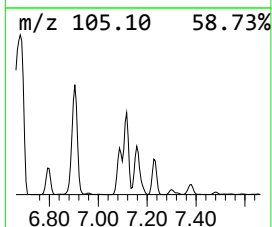
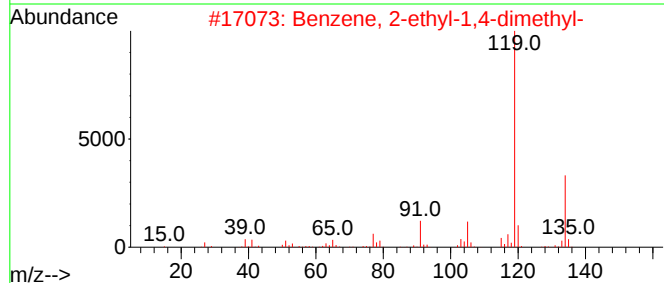
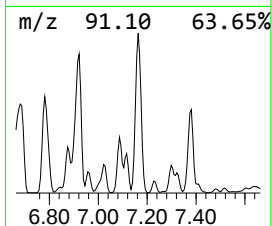
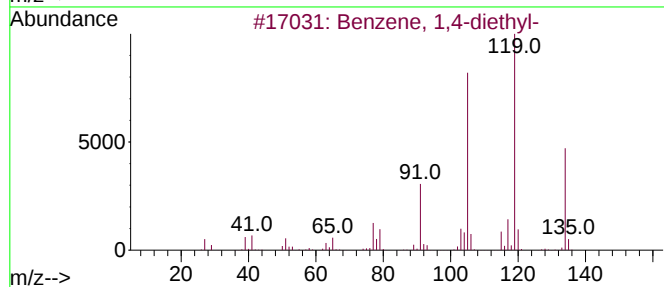
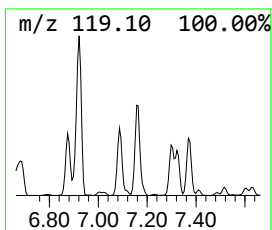
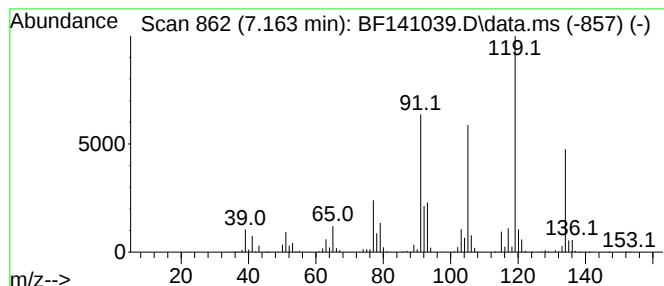
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1,4-diethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	18.02 ng	18493400	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	94
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	92
3			p-Cymene	134	C10H14	000099-87-6	92
4			Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	91
5			o-Cymene	134	C10H14	000527-84-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
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Instrument :
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ClientSampleId :
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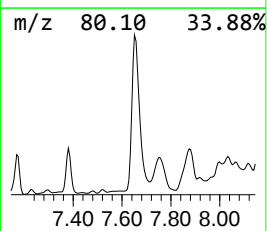
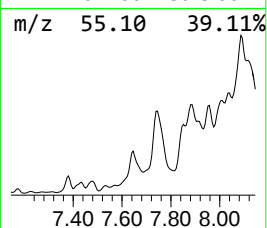
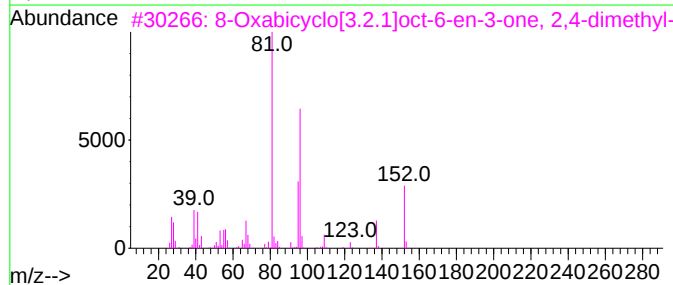
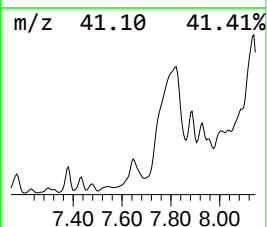
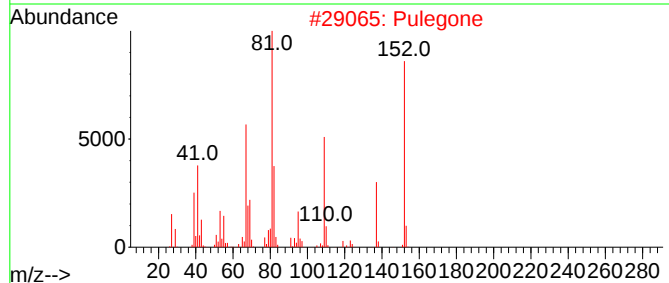
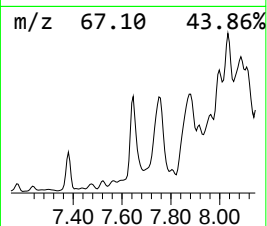
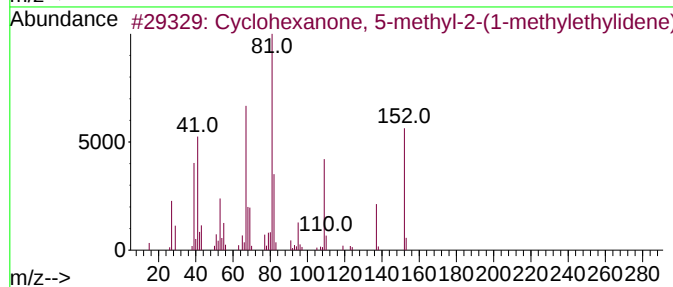
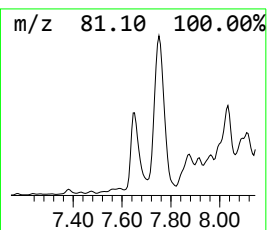
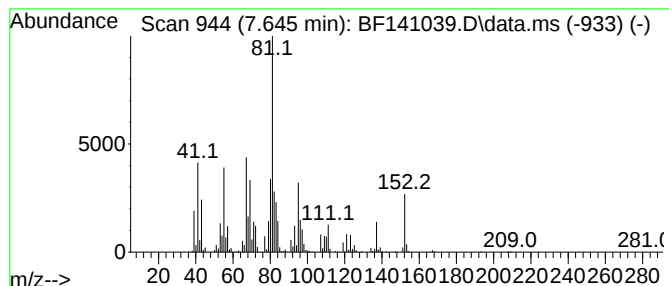
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cyclohexanone, 5-methyl-2-(... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.645	37.71 ng	13729600	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	62
2			Pulegone	152	C10H16O	000089-82-7	58
3			8-Oxabicyclo[3.2.1]oct-6-en-3-on...	152	C9H12O2	049747-05-9	52
4			Cyclohexene, 1-ethyl-	110	C8H14	001453-24-3	43
5			Spiro[4.5]decan-2-one	152	C10H16O	003643-16-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
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Instrument :
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ClientSampleId :
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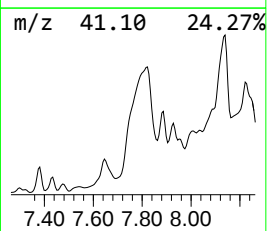
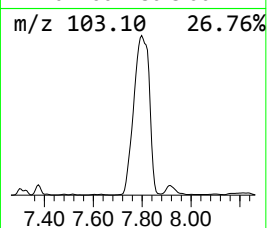
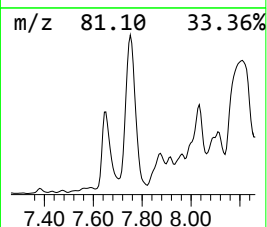
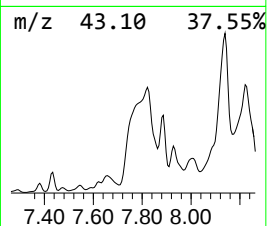
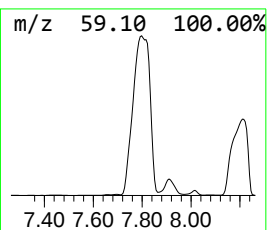
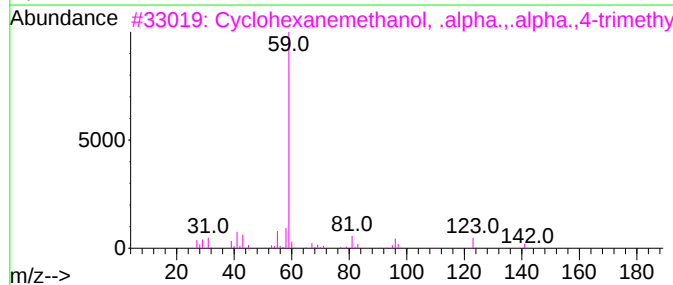
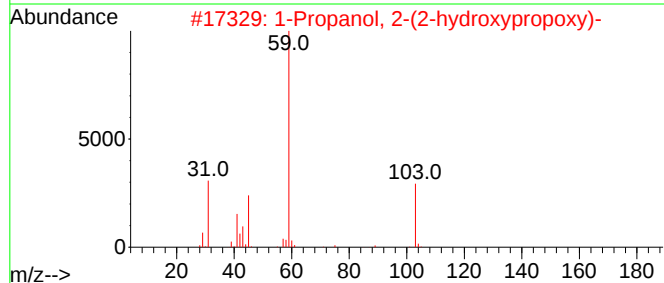
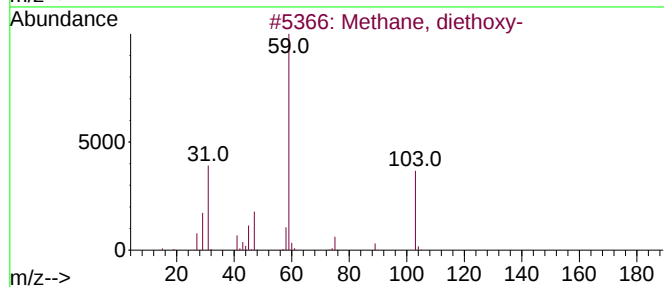
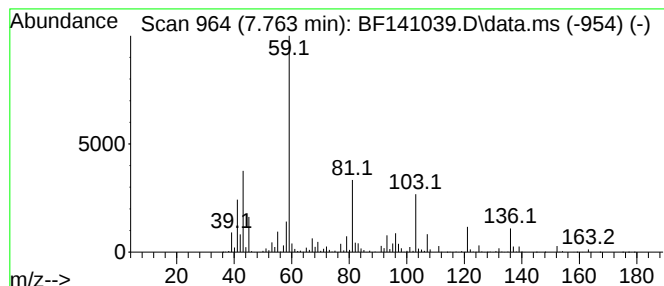
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methane, diethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.763	125.34 ng	45635100	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, diethoxy-	104	C5H12O2	000462-95-3	64
2			1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
3			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	53
4			Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	53
5			Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
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Sample : P5386-01
Misc :
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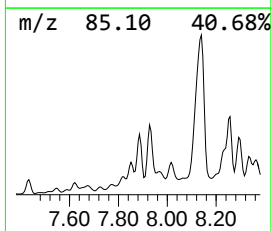
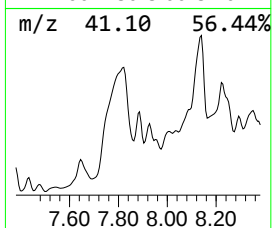
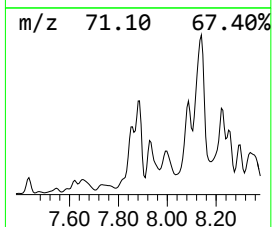
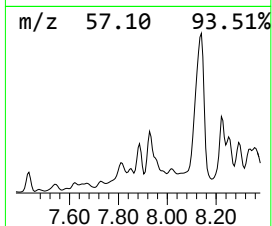
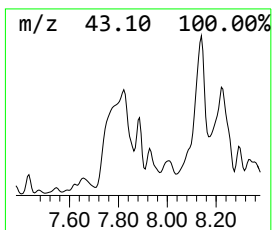
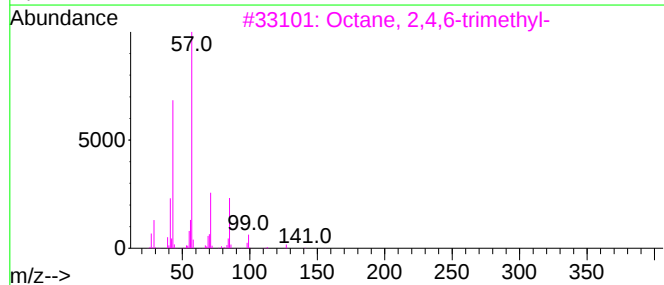
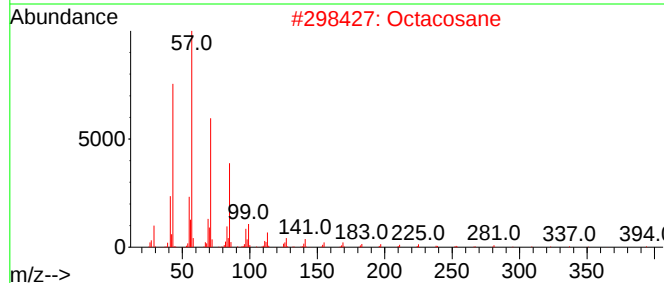
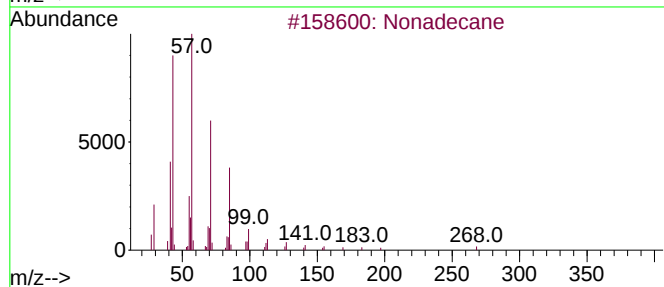
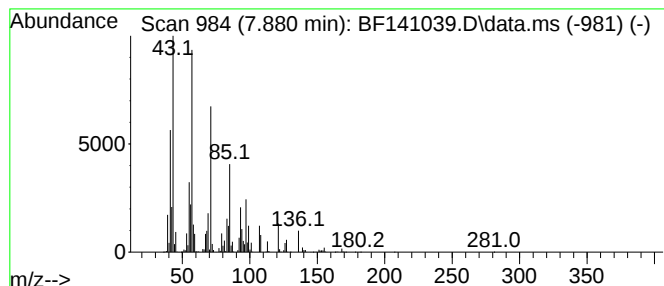
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown7.880 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.880	19.62 ng	7142090	Naphthalene-d8	8.128	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	46
2	Octacosane	394	C28H58	000630-02-4	43
3	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	43
4	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	43
5	Tetradecane	198	C14H30	000629-59-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
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Instrument :
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ClientSampleId :
MOO-24-00398

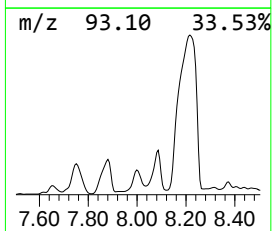
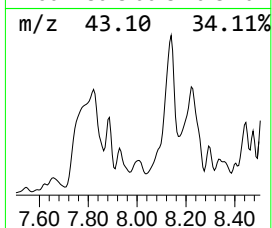
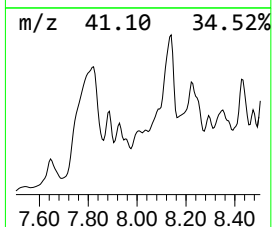
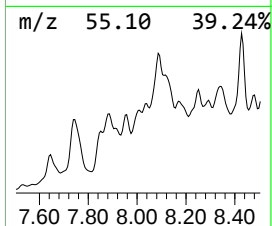
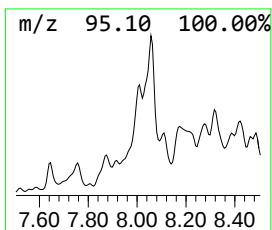
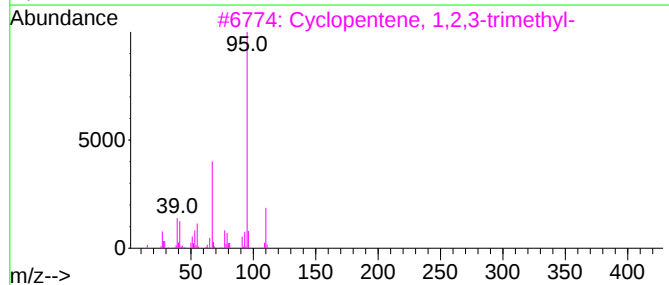
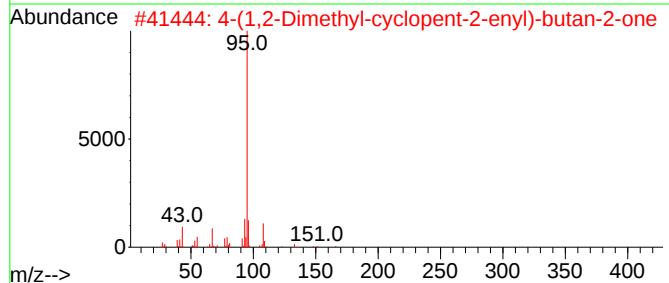
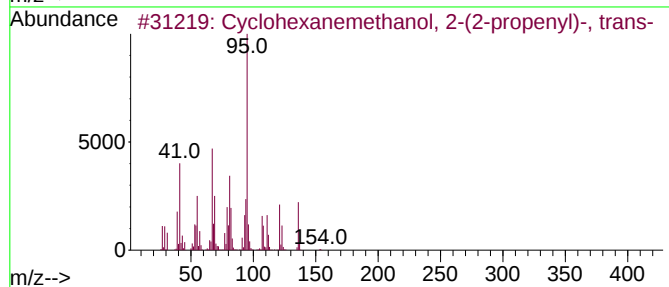
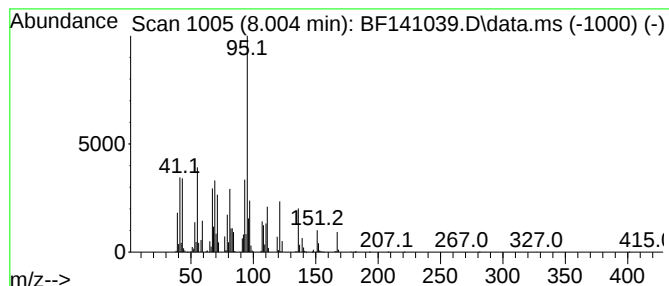
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexanemethanol, 2-(2-p... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	20.00 ng	7281860	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol, 2-(2-propen...	154	C10H18O	134837-38-0	59
2			4-(1,2-Dimethyl-cyclopent-2-enyl...	166	C11H18O	075698-06-5	43
3			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	38
4			2-Furancarboxylic acid, 2-propen...	152	C8H8O3	004208-49-5	38
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
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ClientSampleId :
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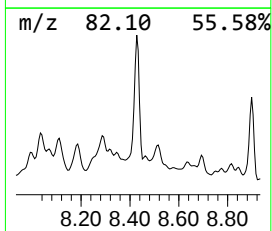
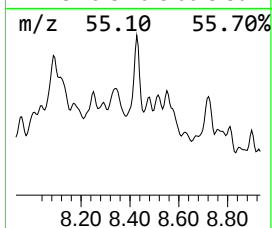
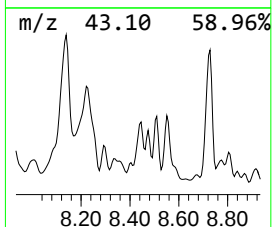
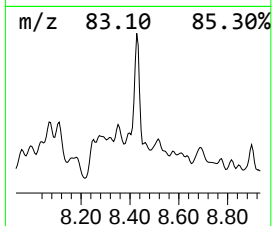
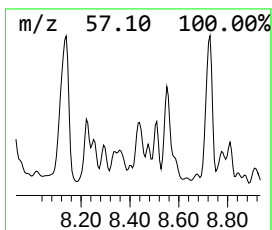
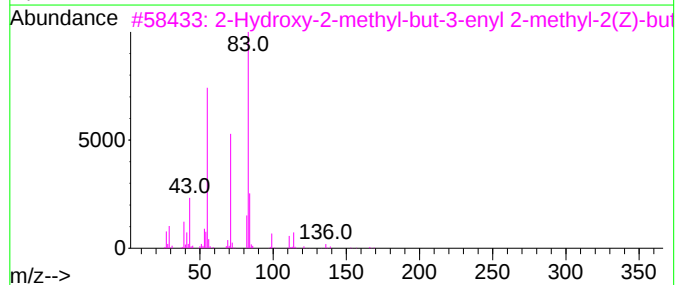
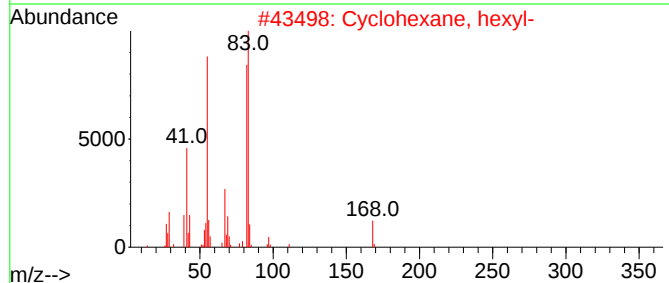
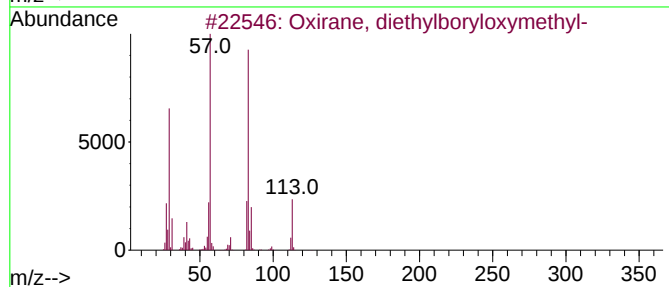
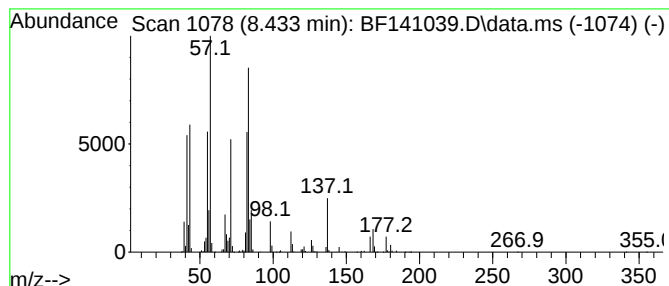
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown8.433 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.433	22.16 ng	8068610	Naphthalene-d8	8.128

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, diethylboryloxymethyl-	142	C7H15BO2	1000161-35-9	47
2		Cyclohexane, hexyl-	168	C12H24	004292-75-5	38
3		2-Hydroxy-2-methyl-but-3-enyl 2-...	184	C10H16O3	080758-67-4	35
4		Propanoic acid, 2,2-dimethyl-, c...	184	C11H20O2	029878-49-7	35
5		(Trimethylsilyl)acetylene	98	C5H10Si	001066-54-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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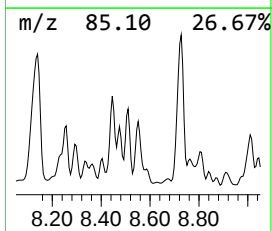
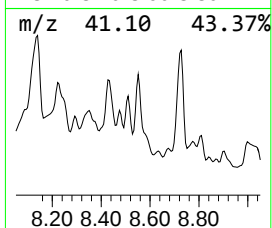
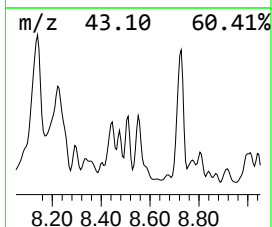
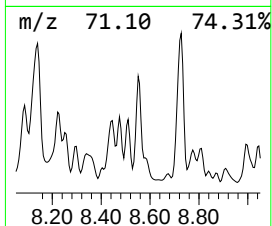
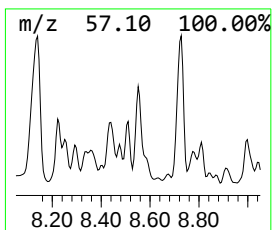
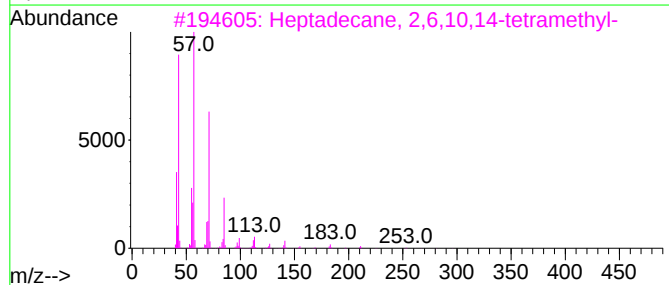
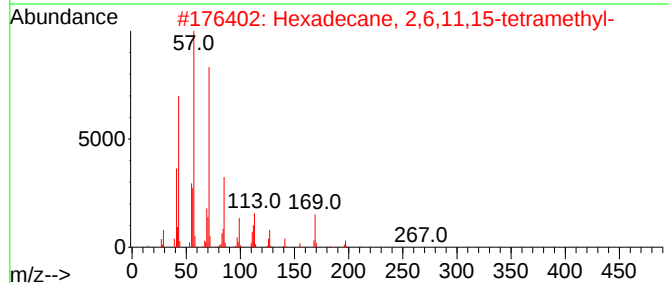
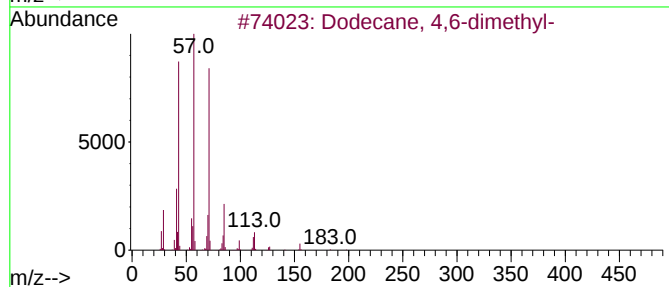
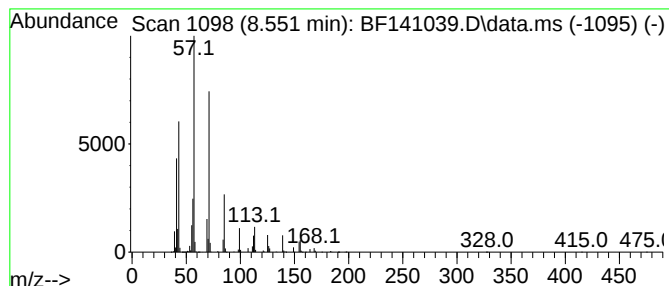
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Dodecane, 4,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	46.16 ng	16806900	Naphthalene-d8	8.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	81
2			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	80
3			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	64
4			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	59
5			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59



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ALS Vial : 10 Sample Multiplier: 1

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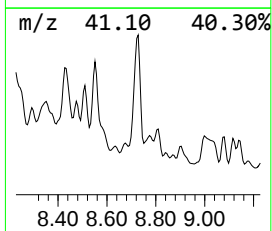
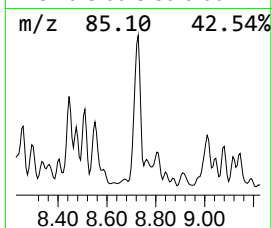
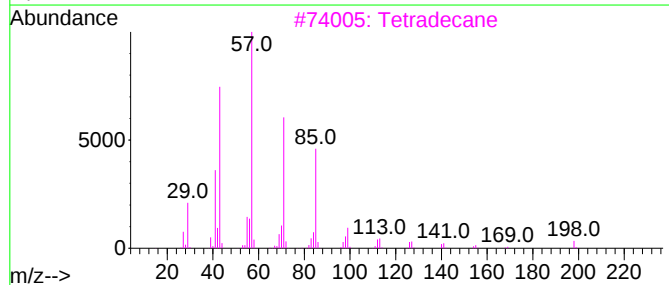
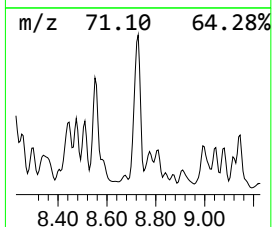
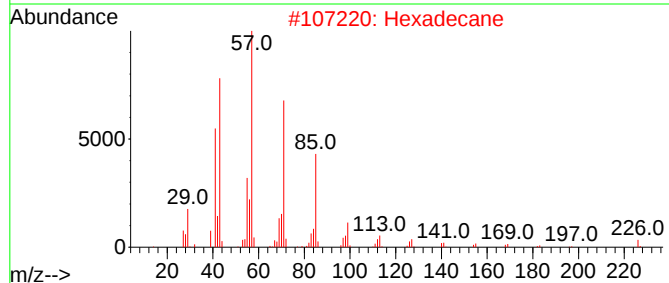
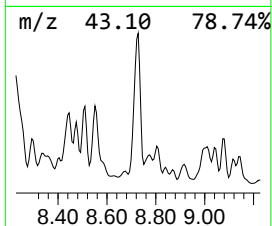
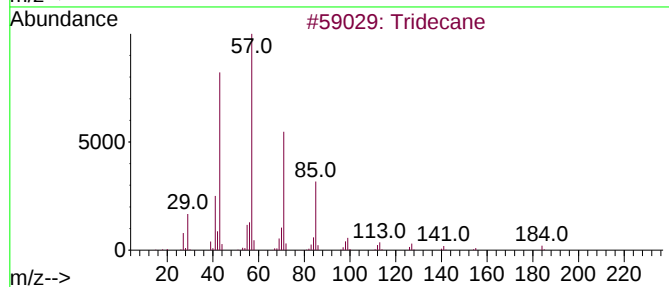
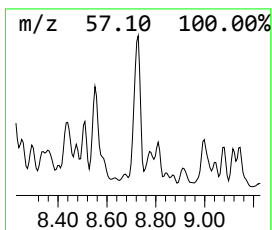
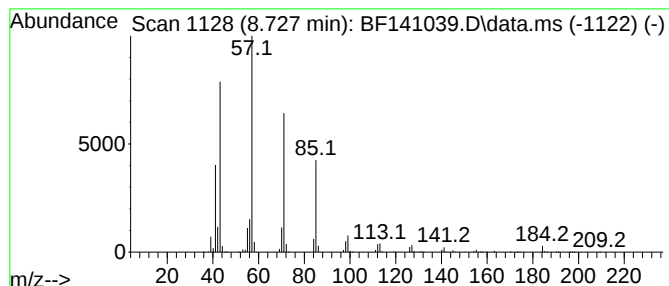
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.727	42.49 ng	15472000	Naphthalene-d8	8.128

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane	184	C13H28	000629-50-5	96
2		Hexadecane	226	C16H34	000544-76-3	91
3		Tetradecane	198	C14H30	000629-59-4	90
4		10-Methylnonadecane	282	C20H42	056862-62-5	86
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
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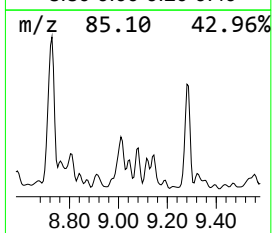
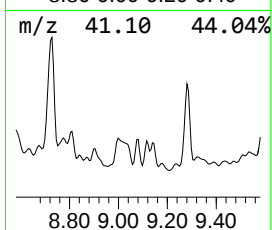
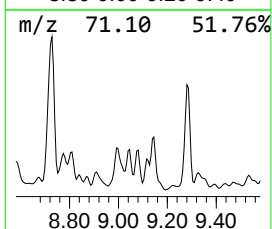
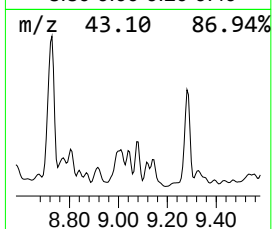
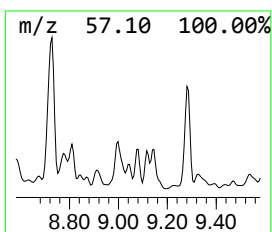
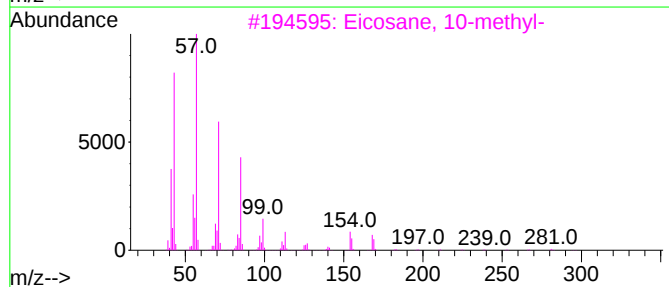
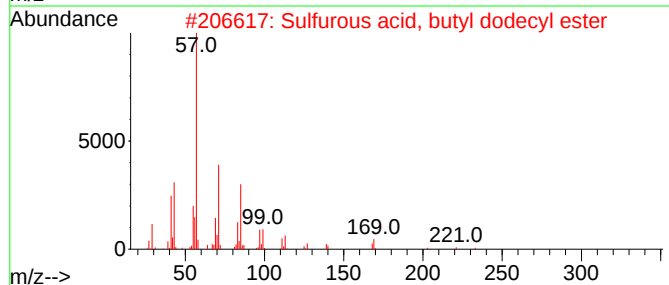
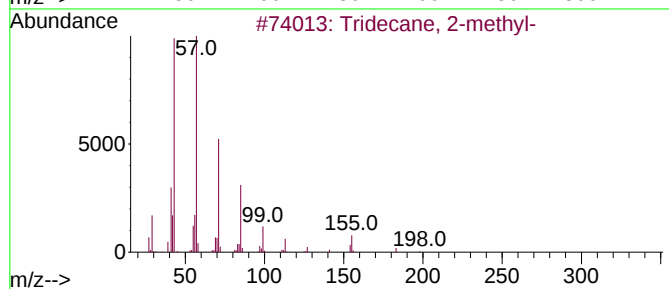
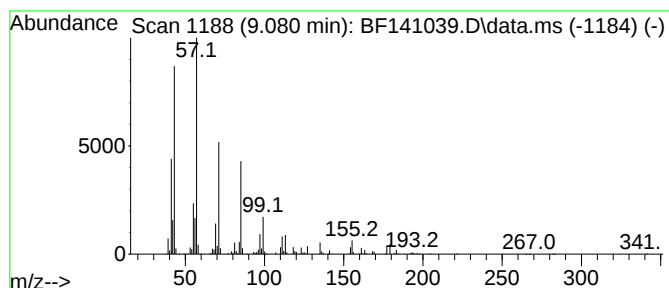
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Tridecane, 2-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.080	17.06 ng	3582880	Acenaphthene-d10	9.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 2-methyl-	198	C14H30	001560-96-9	92
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80
4	Hentriacontane	437	C31H64	000630-04-6	80
5	10-Methylnonadecane	282	C20H42	056862-62-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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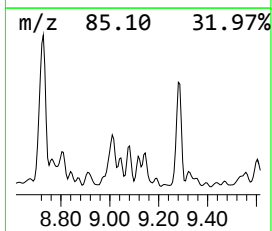
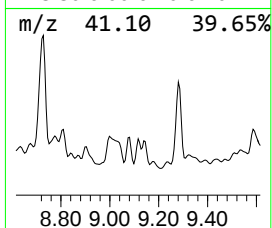
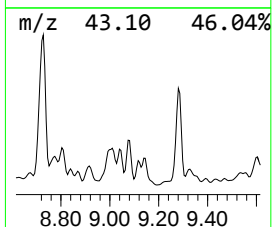
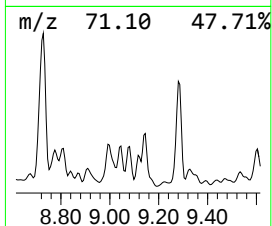
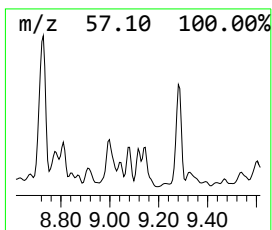
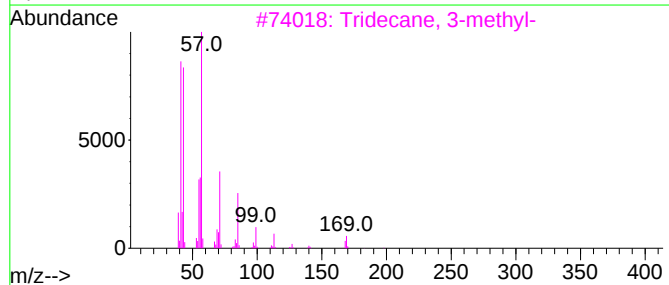
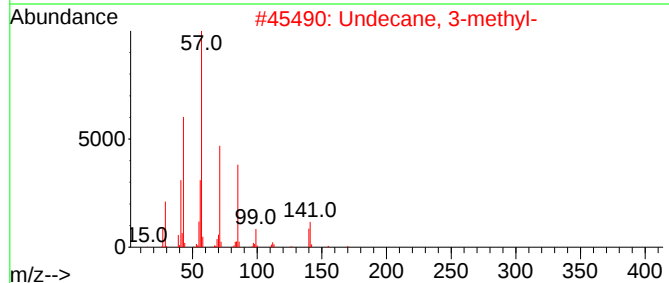
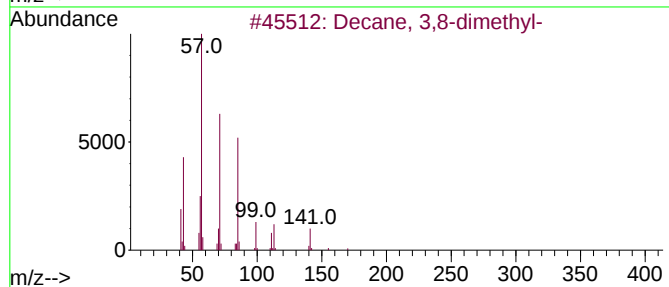
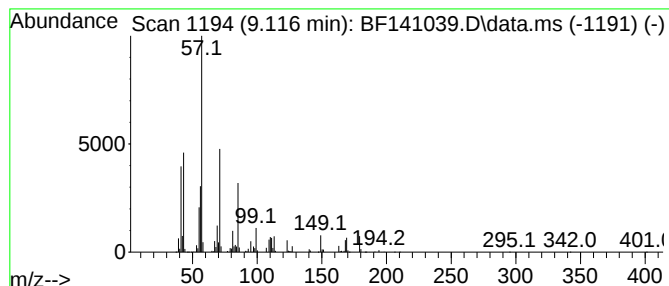
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Decane, 3,8-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.116	13.67 ng	2870560	Acenaphthene-d10	9.874

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	81
2		Undecane, 3-methyl-	170	C12H26	001002-43-3	81
3		Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
4		Dodecane, 3-methyl-	184	C13H28	017312-57-1	64
5		3,5-Dimethyldodecane	198	C14H30	107770-99-0	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
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Operator : RC/JU
Sample : P5386-01
Misc :
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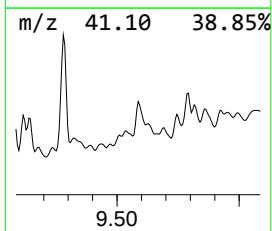
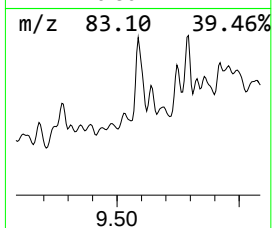
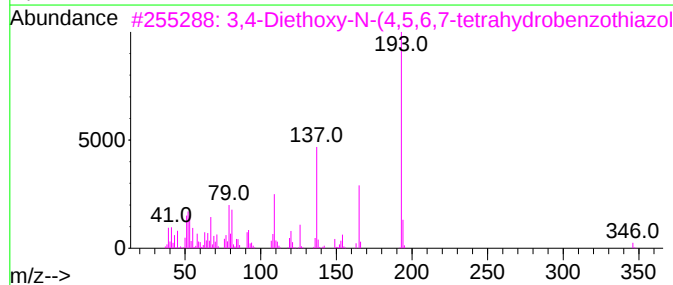
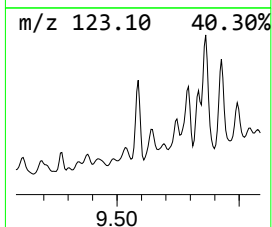
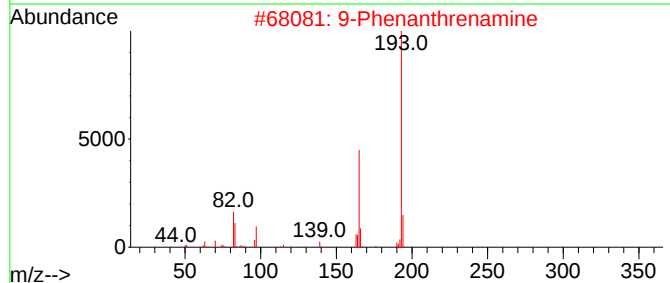
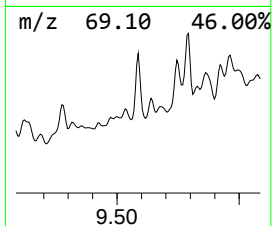
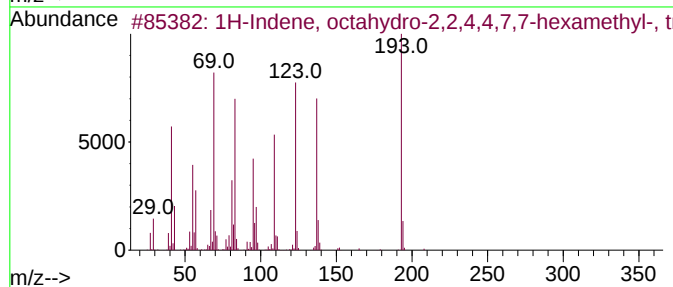
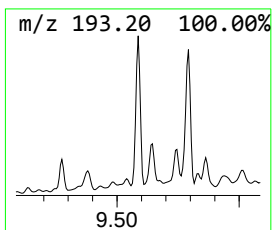
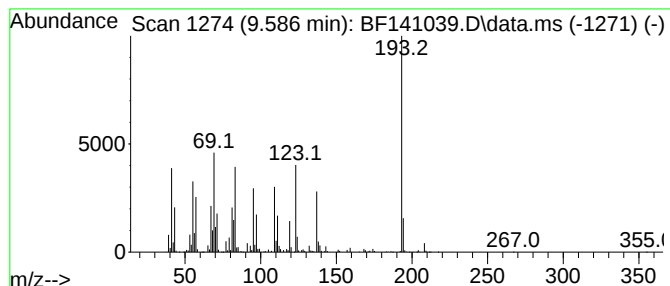
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1H-Indene, octahydro-2,2,4,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.586	31.79 ng	6674010	Acenaphthene-d10	9.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	50
2	9-Phenanthrenamine	193	C14H11N	000947-73-9	27
3	3,4-Diethoxy-N-(4,5,6,7-tetrahyd...	346	C18H22N2O3S	1000311-37-1	25
4	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	23
5	4H-1,3,2-Dioxaborin, 4-ethenyl-2...	208	C12H21BO2	074630-04-9	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
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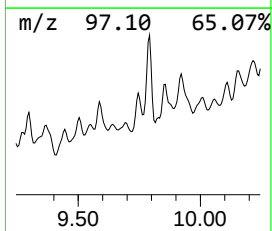
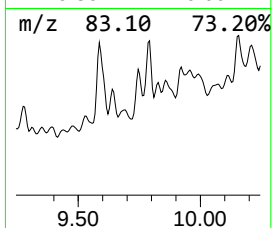
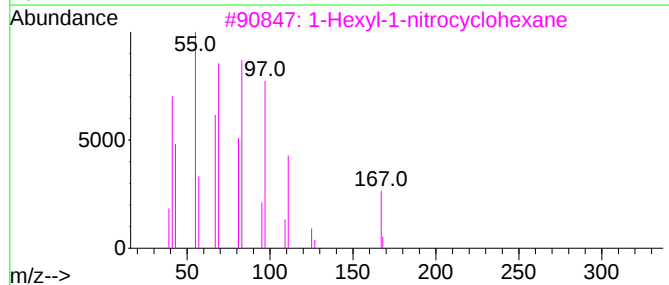
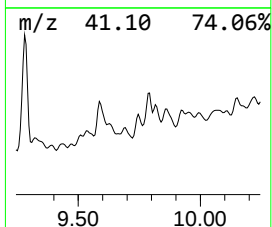
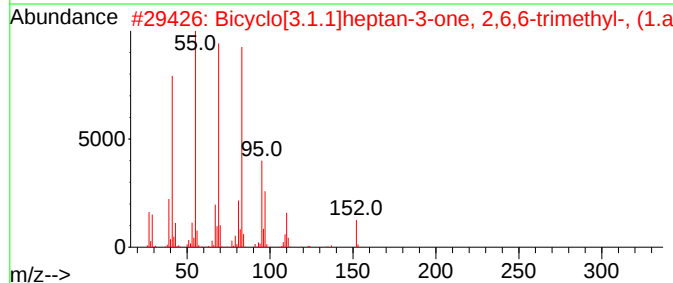
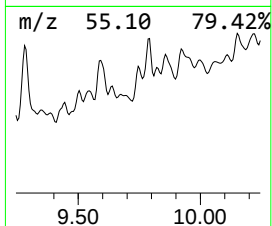
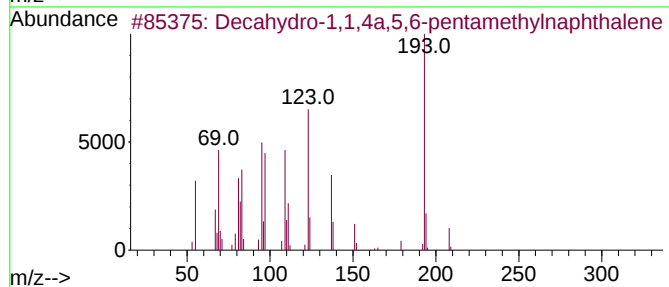
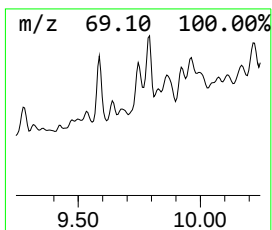
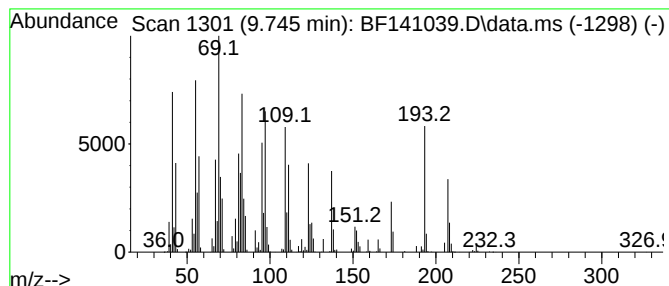
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown9.745 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.745	16.80 ng	3527010	Acenaphthene-d10	9.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	42
2			Bicyclo[3.1.1]heptan-3-one, 2,6,...	152	C10H16O	000547-60-4	38
3			1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	35
4			(S)-3-(4-Fluorobenzyl)piperidine	193	C12H16FN	275815-80-0	27
5			Octadienyl angelate, 2E, 4E-	208	C13H20O2	1000383-60-4	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
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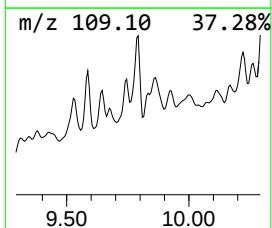
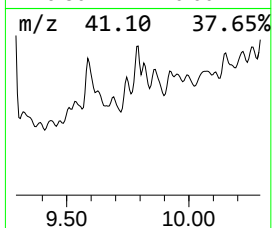
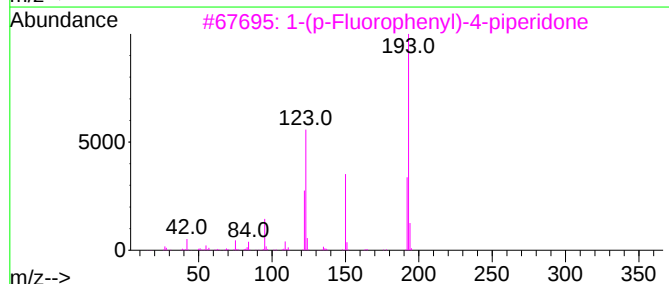
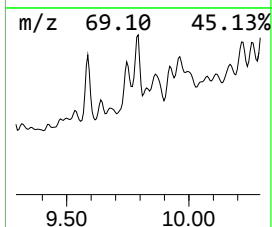
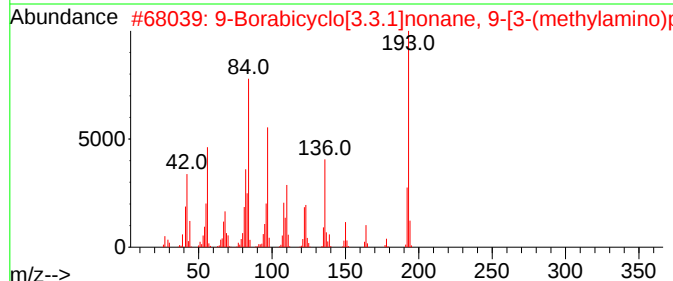
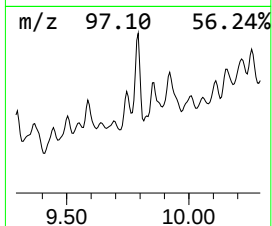
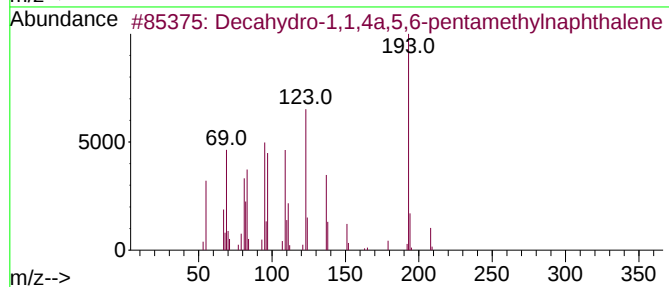
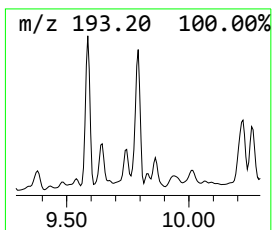
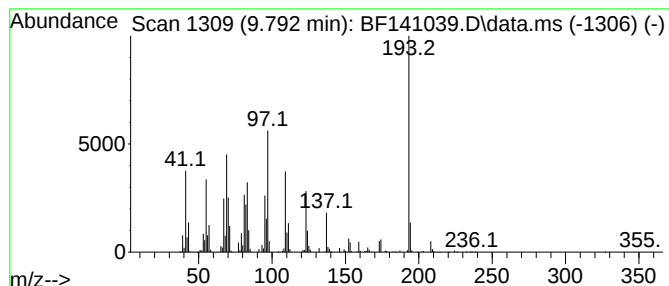
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ClientSampleId :
MOO-24-00398

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.792	18.23 ng	3827390	Acenaphthene-d10		9.874	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	50
2	9-Borabicyclo[3.3.1]nonane, 9-[3...		193	C12H24BN	1010162-56-0	50
3	1-(p-Fluorophenyl)-4-piperidone		193	C11H12FNO	1000238-56-7	38
4	Benzonitrile, pentafluoro-		193	C7F5N	000773-82-0	35
5	Acridine, 9-methyl-		193	C14H11N	000611-64-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

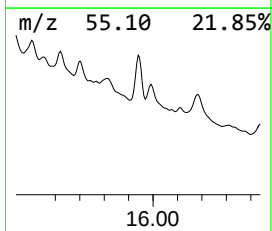
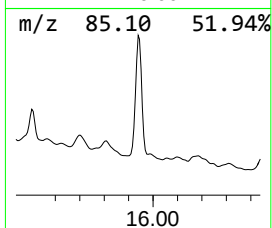
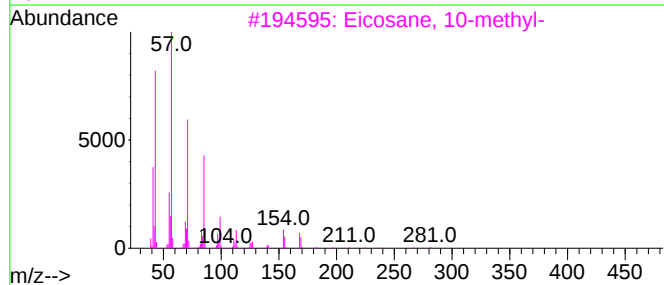
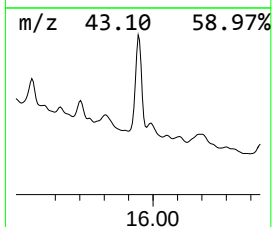
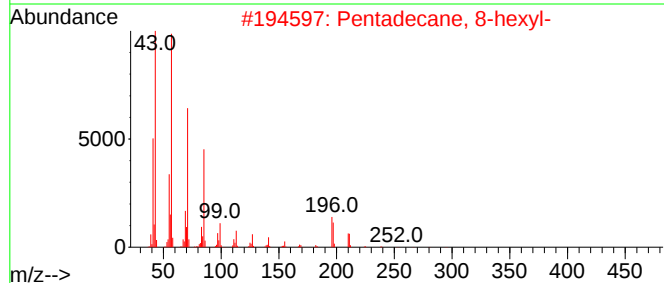
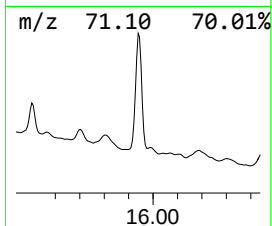
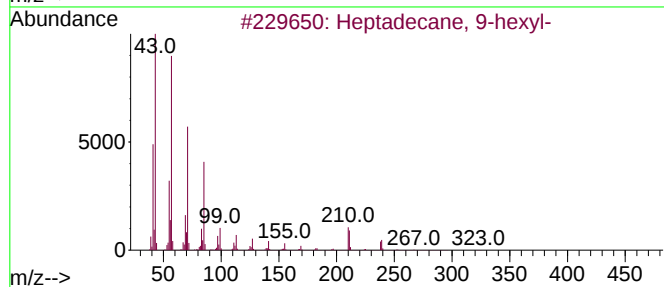
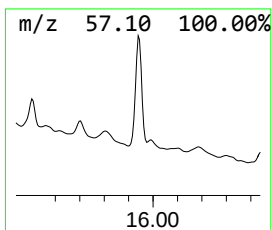
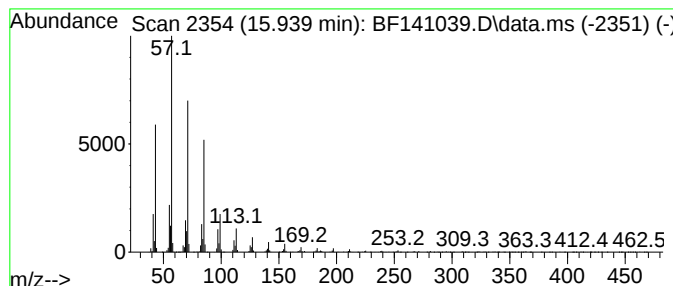
Instrument :
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ClientSampleId :
MOO-24-00398

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Heptadecane, 9-hexyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.939	20.00 ng	1548440	Perylene-d12	15.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4	Octacosane	394	C28H58	000630-02-4	91
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-24-00398

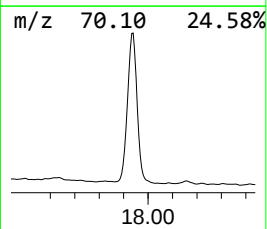
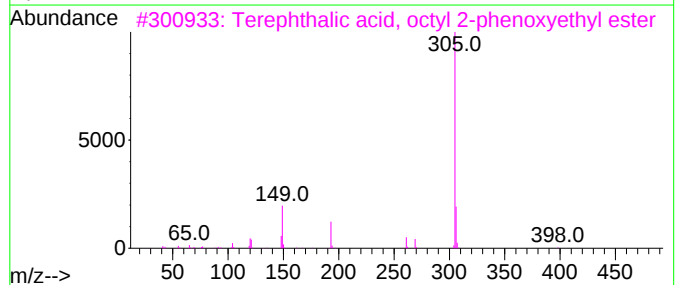
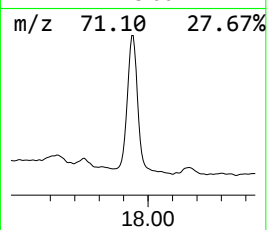
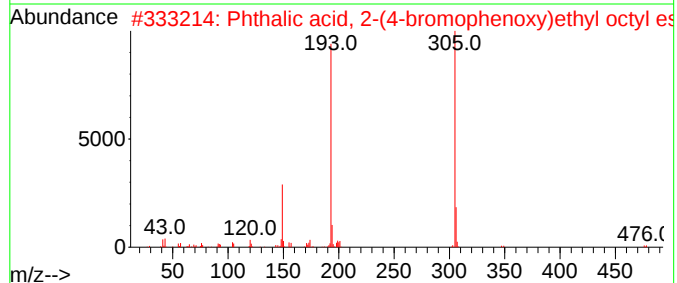
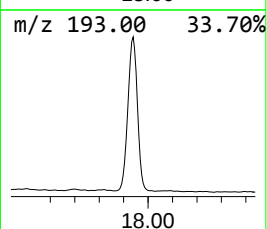
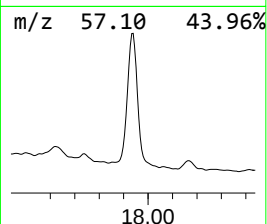
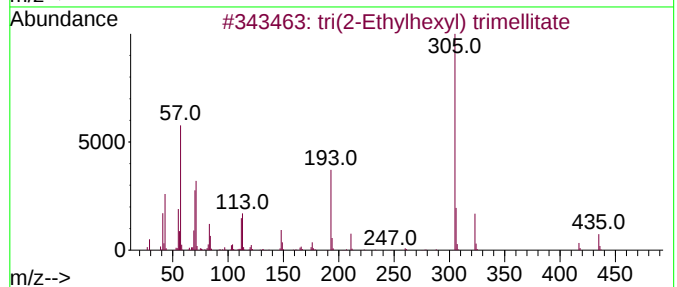
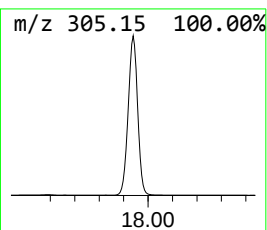
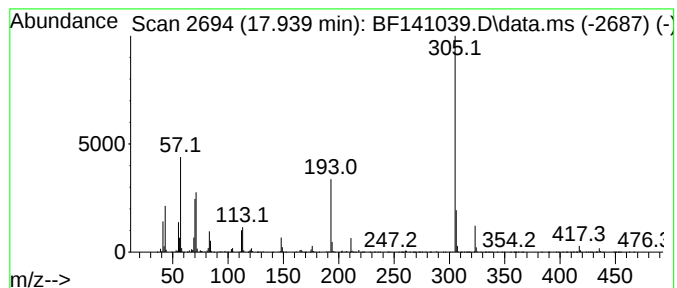
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 tri(2-Ethylhexyl) trimellitate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.939	43.72 ng	3384750	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			tri(2-Ethylhexyl) trimellitate	546	C33H54O6	003319-31-1	58
2			Phthalic acid, 2-(4-bromophenoxy)ethyl octyl ester	476	C24H29BrO5	1010382-89-7	53
3			Terephthalic acid, octyl 2-phenoxyethyl ester	398	C24H30O5	1000416-04-7	38
4			4-(Diphenylphosphino)-N,N-dimethyl-1-piperazine	305	C20H20NP	000739-58-2	37
5			Benzeneacetamide, N-[5-methyl-1-piperazinyl]	305	C19H19N3O	1000337-48-2	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF123024\
Data File : BF141039.D
Acq On : 30 Dec 2024 18:58
Operator : RC/JU
Sample : P5386-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MOO-24-00398

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122624.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
2-Pentanone, 4-...	5.169	80.3	ng	82353200	1	6.839	20524200	20.0
Benzene, 1-ethy...	6.375	28.4	ng	29089600	1	6.839	20524200	20.0
Benzene, 1,2,3-...	6.681	38.3	ng	39325700	1	6.839	20524200	20.0
Mesitylene	6.910	26.3	ng	27023500	1	6.839	20524200	20.0
Eucalyptol	7.004	21.0	ng	21582000	1	6.839	20524200	20.0
Benzene, 1,4-di...	7.163	18.0	ng	18493400	1	6.839	20524200	20.0
Cyclohexanone, ...	7.645	37.7	ng	13729600	2	8.128	7281860	20.0
Methane, diethoxy-	7.763	125.3	ng	45635100	2	8.128	7281860	20.0
unknown7.880	7.880	19.6	ng	7142090	2	8.128	7281860	20.0
Cyclohexanemeth...	8.004	20.0	ng	7281860	2	8.128	7281860	20.0
unknown8.433	8.433	22.2	ng	8068610	2	8.128	7281860	20.0
Dodecane, 4,6-d...	8.551	46.2	ng	16806900	2	8.128	7281860	20.0
Tridecane	8.727	42.5	ng	15472000	2	8.128	7281860	20.0
Tridecane, 2-me...	9.080	17.1	ng	3582880	3	9.874	4199240	20.0
Decane, 3,8-dim...	9.116	13.7	ng	2870560	3	9.874	4199240	20.0
1H-Indene, octa...	9.586	31.8	ng	6674010	3	9.874	4199240	20.0
unknown9.745	9.745	16.8	ng	3527010	3	9.874	4199240	20.0
Decahydro-1,1,4...	9.792	18.2	ng	3827390	3	9.874	4199240	20.0
Heptadecane, 9-...	15.939	20.0	ng	1548440	6	15.468	1548440	20.0
tri(2-Ethylhexy...	17.939	43.7	ng	3384750	6	15.468	1548440	20.0