

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012023\
 Data File : BF132167.D
 Acq On : 20 Jan 2023 18:23
 Operator : CG\JU
 Sample : 01160-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-04-SB02

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-BF011923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132167.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.284	242	246	250	rVB	113169	132289	3.52%	0.405%
2	5.331	414	424	431	rBV	1202851	1387729	36.94%	4.249%
3	5.595	466	469	473	rBV	58324	53140	1.41%	0.163%
4	5.713	484	489	492	rBV	2906423	3002287	79.92%	9.193%
5	6.695	651	656	659	rBV	2963706	3034395	80.77%	9.292%
6	7.089	719	723	726	rBV	1350729	1055022	28.08%	3.231%
7	7.648	814	818	821	rBV	2213676	1936713	51.55%	5.930%
8	8.378	938	942	945	rBV	1583472	1353982	36.04%	4.146%
9	9.454	1121	1125	1128	rVB	4030010	3455078	91.97%	10.580%
10	9.519	1133	1136	1139	rBV	50562	41313	1.10%	0.127%
11	9.595	1146	1149	1151	rBV2	47625	45013	1.20%	0.138%
12	9.683	1161	1164	1167	rBV	66254	52925	1.41%	0.162%
13	9.795	1180	1183	1188	rVV	1168316	953252	25.37%	2.919%
14	9.848	1188	1192	1195	rVV2	208844	198578	5.29%	0.608%
15	9.878	1195	1197	1198	rVV	118408	93013	2.48%	0.285%
16	9.895	1198	1200	1203	rVB	176061	137397	3.66%	0.421%
17	9.936	1203	1207	1210	rBV	132342	103631	2.76%	0.317%
18	10.007	1216	1219	1224	rBV	793934	708764	18.87%	2.170%
19	10.048	1224	1226	1229	rVB2	49390	40849	1.09%	0.125%
20	10.142	1235	1242	1249	rBV2	1926899	2462464	65.55%	7.540%
21	10.266	1259	1263	1270	rVB	600576	616563	16.41%	1.888%
22	10.383	1280	1283	1285	rBV	47229	43274	1.15%	0.133%
23	10.413	1285	1288	1292	rVB	131087	116978	3.11%	0.358%
24	10.854	1360	1363	1366	rBV	637139	465639	12.39%	1.426%
25	10.930	1372	1376	1380	rBV	2715948	2501386	66.58%	7.660%
26	11.642	1493	1497	1500	rBV	1755953	1638290	43.61%	5.017%
27	12.148	1576	1583	1587	rBV	446341	428738	11.41%	1.313%
28	12.936	1713	1717	1724	rBV	122110	120662	3.21%	0.369%
29	13.230	1763	1767	1771	rBV	3894809	3756780	100.00%	11.504%
30	14.130	1917	1920	1922	rBV2	85351	104357	2.78%	0.320%
31	14.265	1940	1943	1945	rVV	56340	45583	1.21%	0.140%
32	14.301	1945	1949	1953	rVB	1572837	1335191	35.54%	4.089%
33	15.483	2146	2150	2156	rVB	37629	46837	1.25%	0.143%
34	15.895	2214	2220	2231	rBV2	743435	1082375	28.81%	3.314%
35	16.995	2402	2407	2415	rBV4	23690	50728	1.35%	0.155%
36	17.530	2494	2498	2505	rVB8	25862	55620	1.48%	0.170%

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Instrument :
BNA_F
ClientSampleId :
B-04-SB02

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-BF011923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

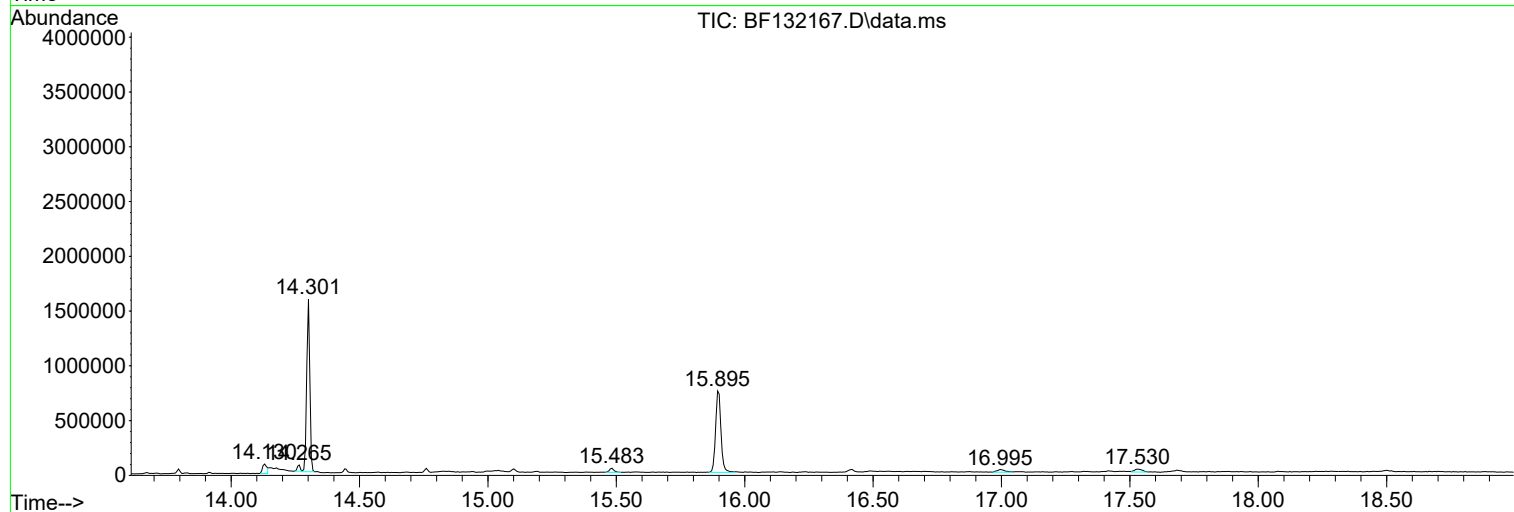
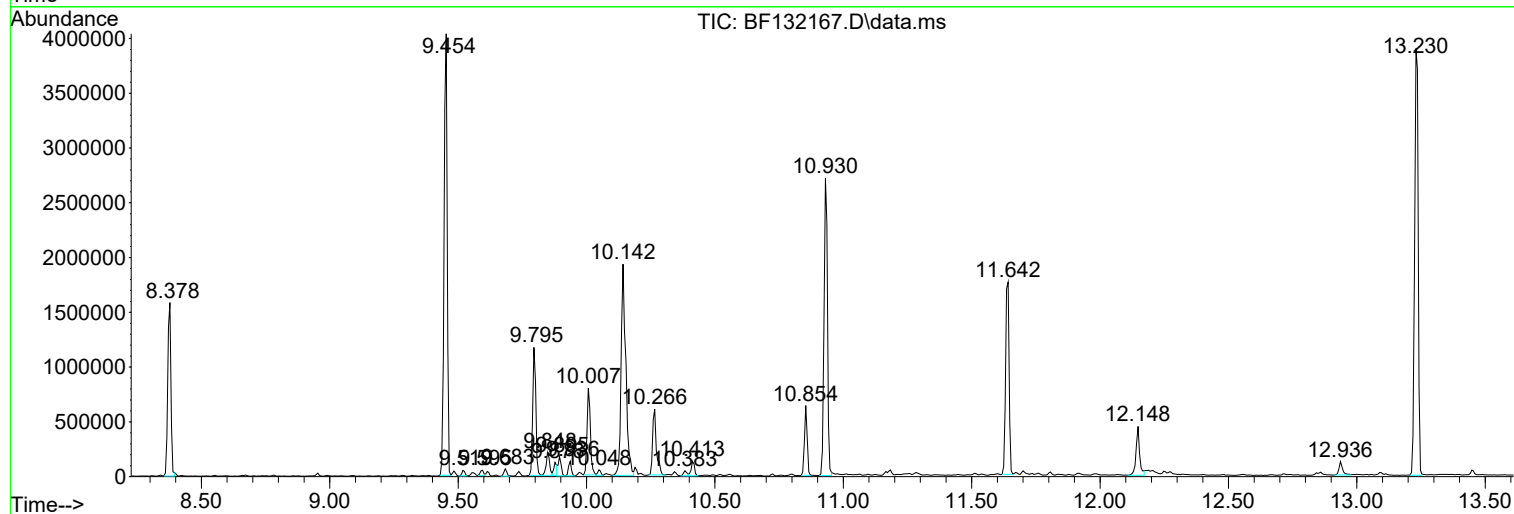
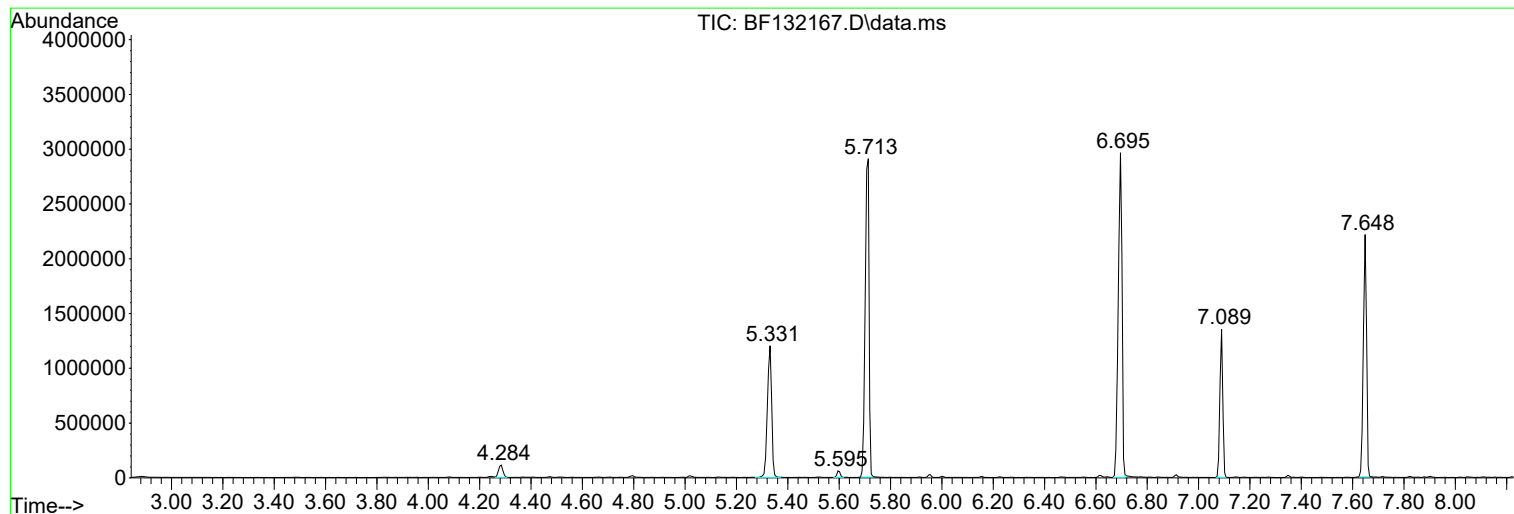
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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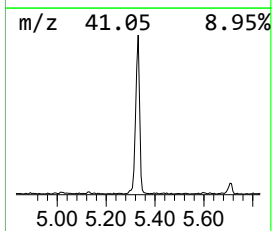
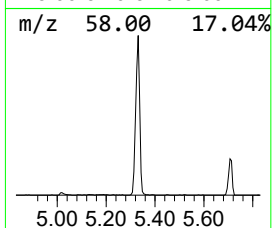
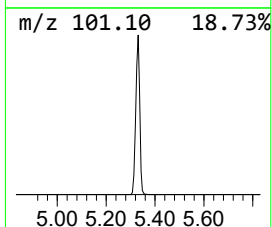
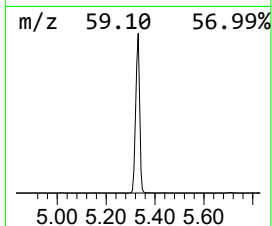
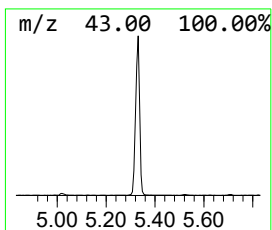
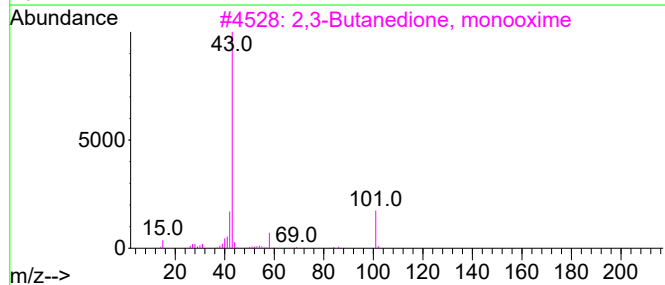
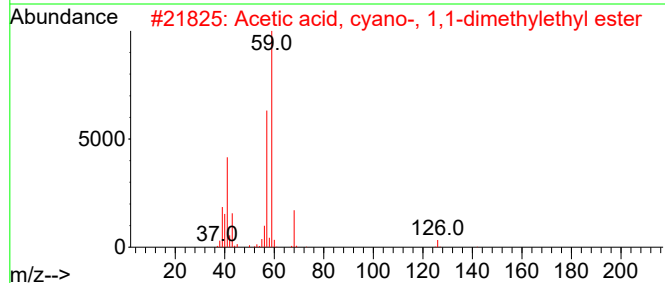
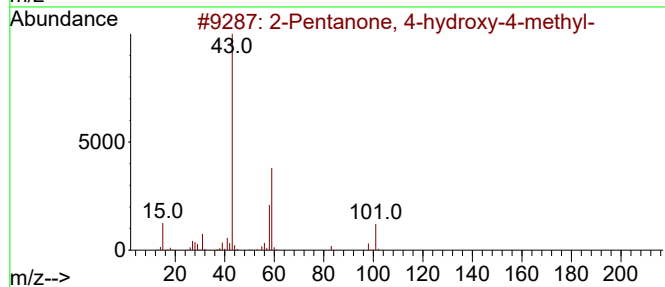
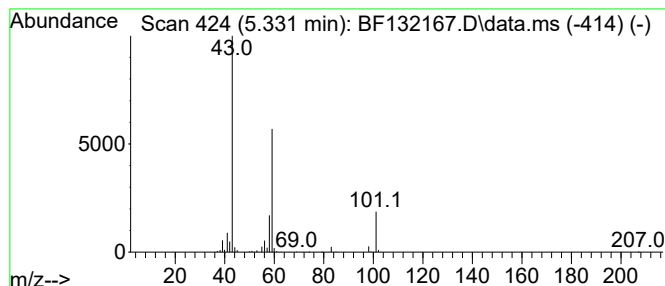
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.331	26.31 ng	1387730	1,4-Dichlorobenzene-d4	7.089

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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Sample : 01160-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

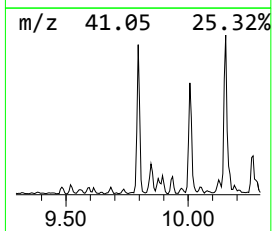
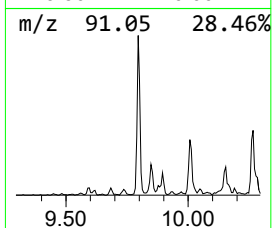
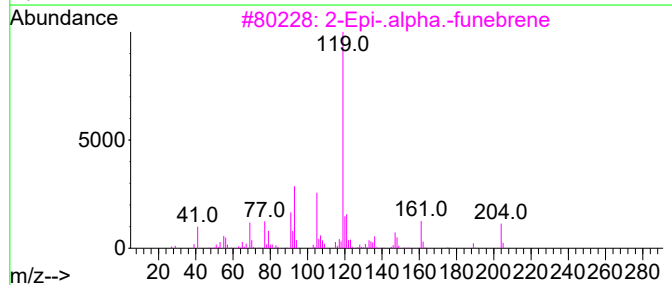
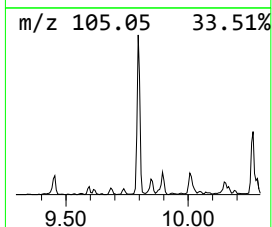
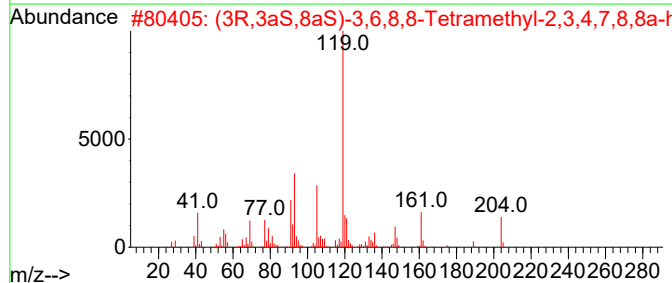
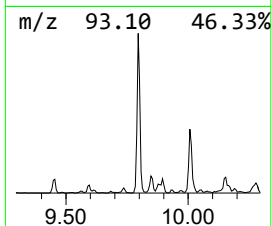
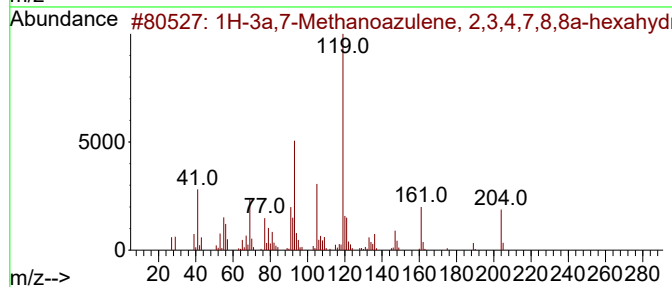
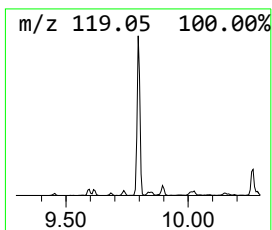
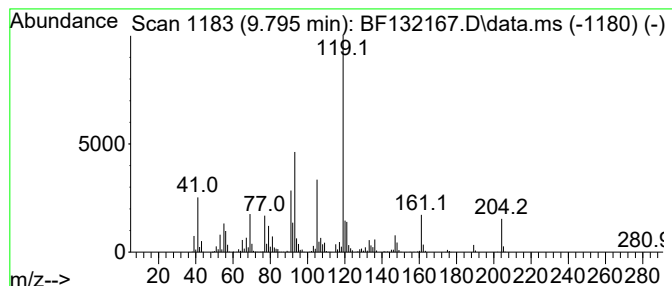
Instrument :
BNA_F
ClientSampleId :
B-04-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1H-3a,7-Methanoazulene, 2,3... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.795	7.74 ng	953252	Acenaphthene-d10	10.142	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,4,7,...	204	C15H24	000469-61-4	98
2	(3R,3aS,8aS)-3,6,8,8-Tetramethyl...	204	C15H24	022567-43-7	98
3	2-Epi-.alpha.-funebrene	204	C15H24	065354-33-8	93
4	(R)-1-Methyl-4-(6-methylhept-5-e...	204	C15H24	028976-67-2	86
5	1,3-Cyclohexadiene, 5-(1,5-dimet...	204	C15H24	000495-60-3	81



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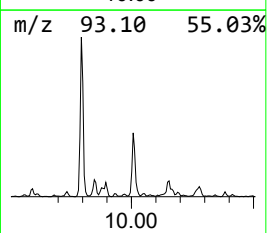
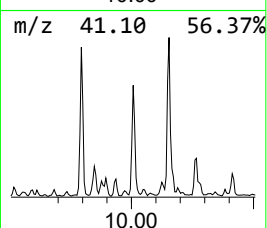
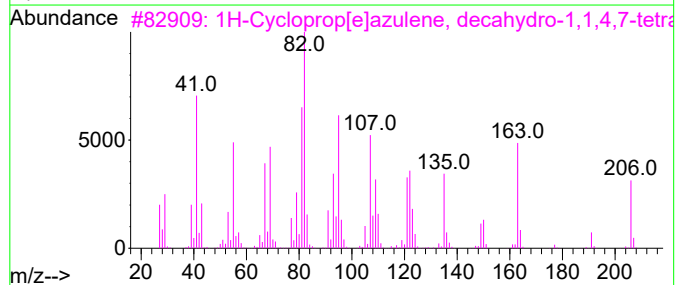
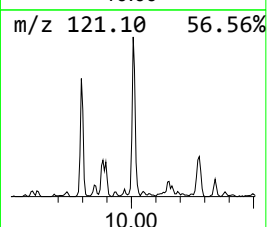
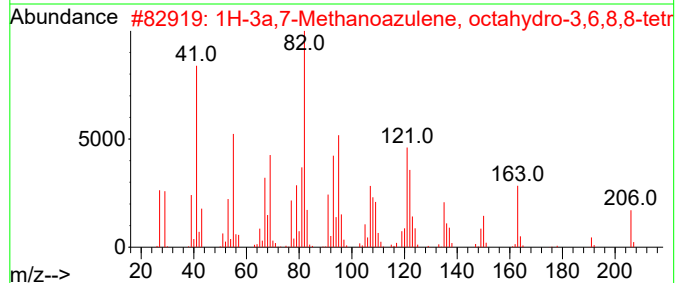
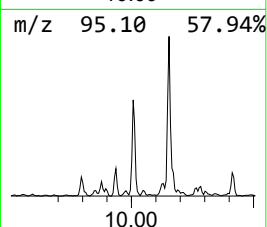
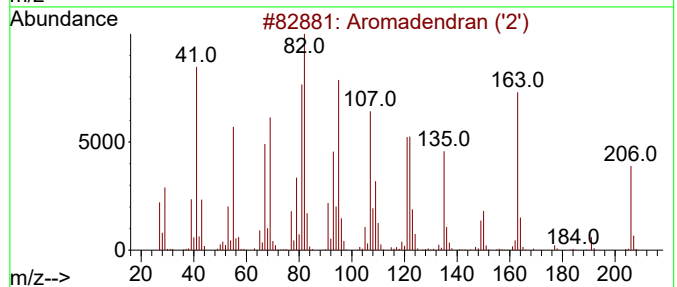
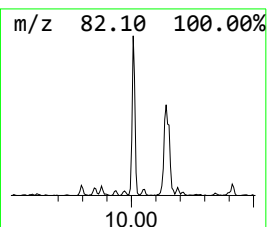
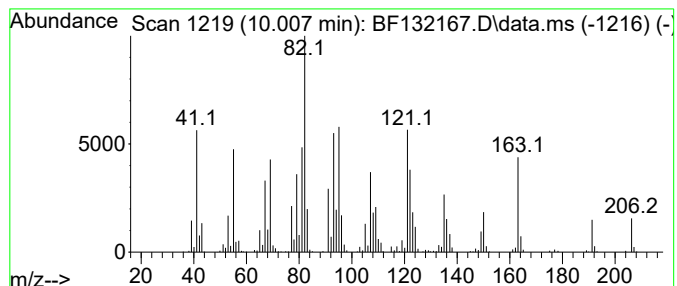
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Aromadendran ('2') Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.007	5.76 ng	708764	Acenaphthene-d10	10.142

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aromadendran ('2')	206	C15H26	110769-62-5	96
2			1H-3a,7-Methanoazulene, octahydr...	206	C15H26	013567-54-9	81
3			1H-Cycloprop[e]azulene, decahydr...	206	C15H26	006790-78-9	76
4			4,7-Methanoazulene, decahydro-1,...	206	C15H26	020478-88-0	62
5			1H-3a,7-Methanoazulene, octahydr...	206	C15H26	003724-42-3	46



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Misc :
ALS Vial : 5 Sample Multiplier: 1

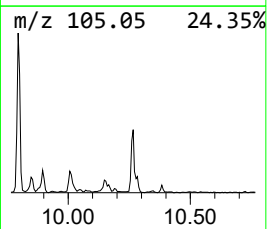
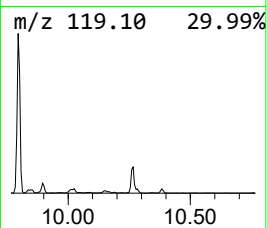
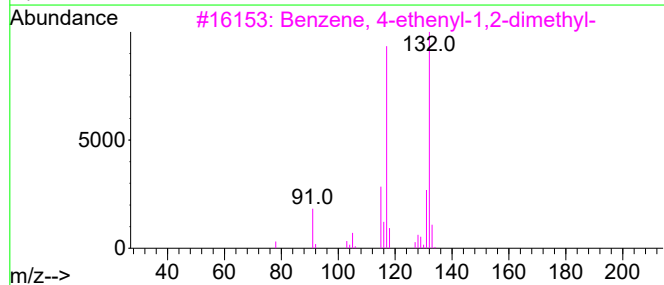
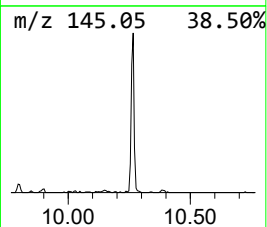
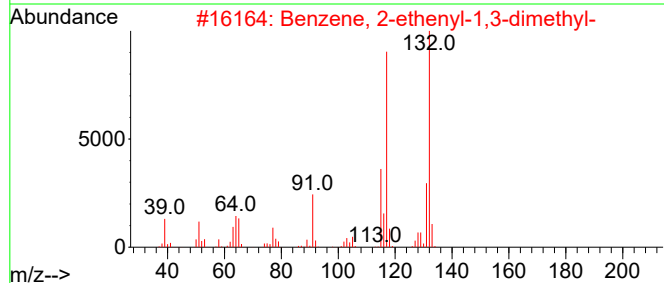
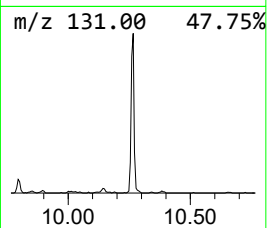
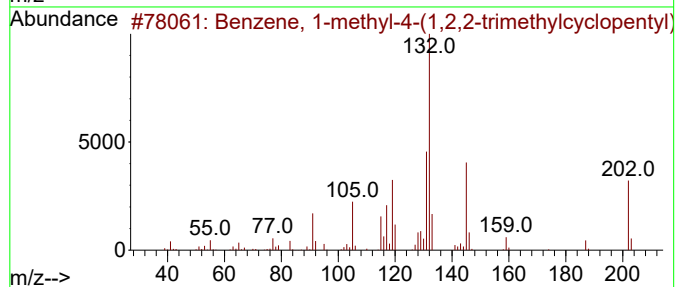
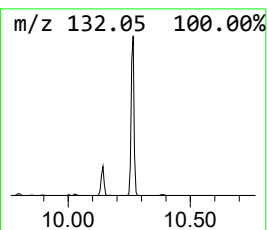
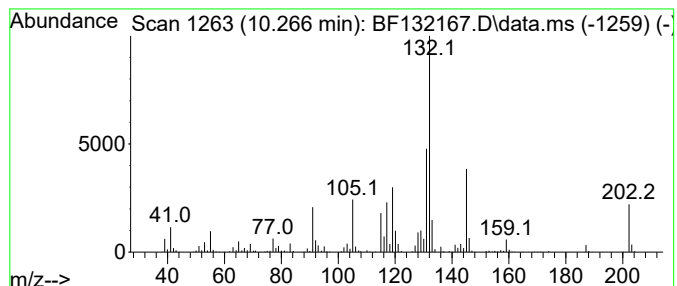
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1-methyl-4-(1,2,2-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.266	5.01 ng	616563	Acenaphthene-d10		10.142	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-4-(1,2,2-trime...		202	C15H22	016982-00-6	99
2	Benzene, 2-ethenyl-1,3-dimethyl-		132	C10H12	002039-90-9	43
3	Benzene, 4-ethenyl-1,2-dimethyl-		132	C10H12	027831-13-6	43
4	5-Methylimidazo[1,2-a]pyridine		132	C8H8N2	000933-69-7	38
5	1-Methylbenzimidazole		132	C8H8N2	001632-83-3	38



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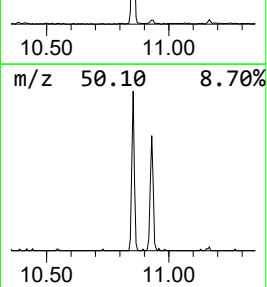
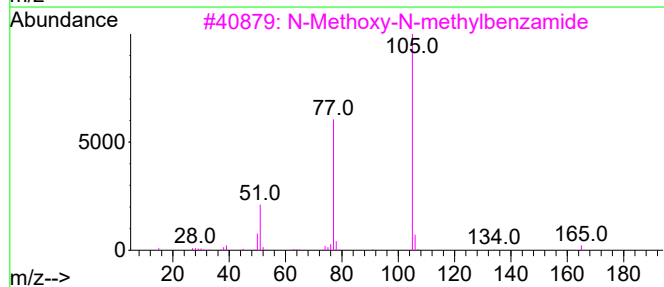
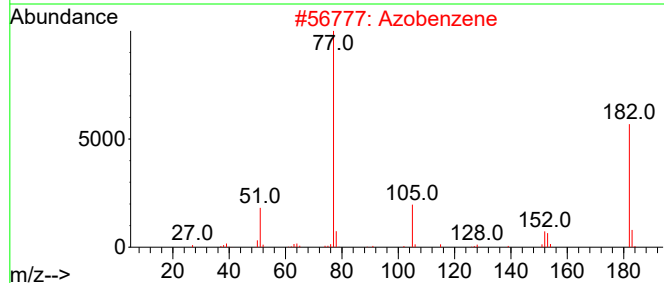
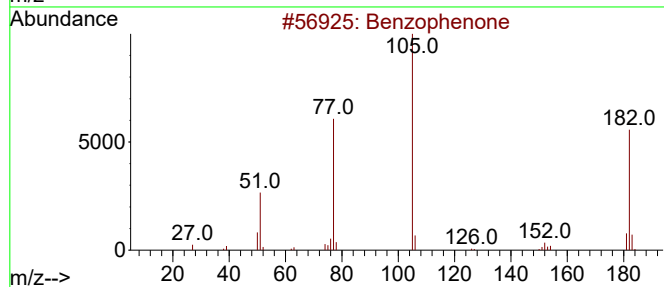
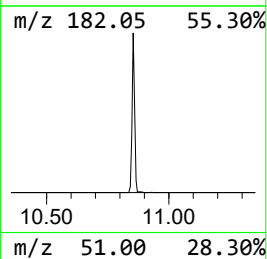
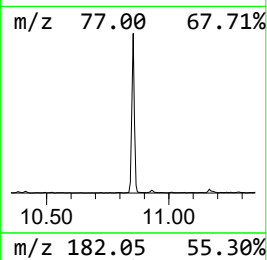
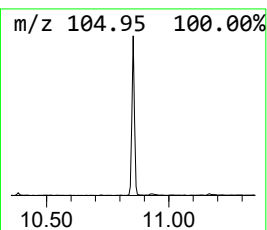
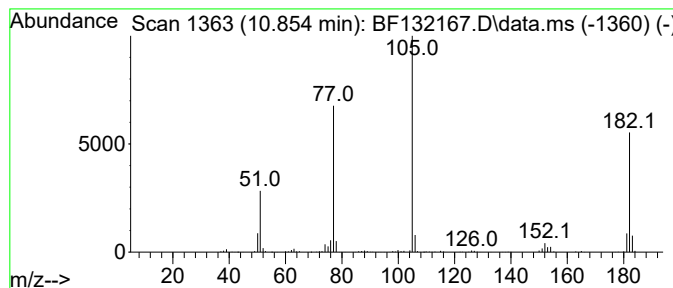
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	3.78 ng	465639	Acenaphthene-d10	10.142

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
4			Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012023\
Data File : BF132167.D
Acq On : 20 Jan 2023 18:23
Operator : CG\JU
Sample : 01160-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-04-SB02

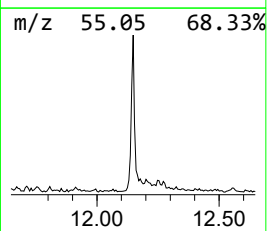
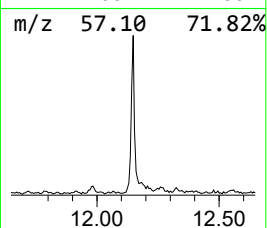
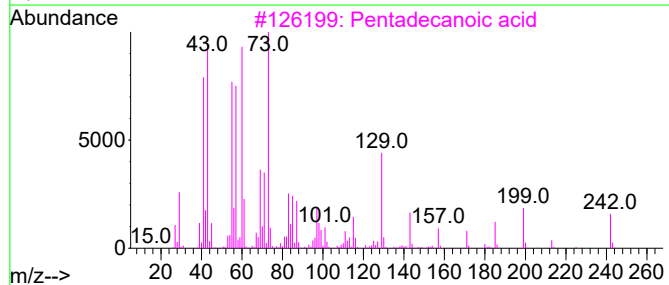
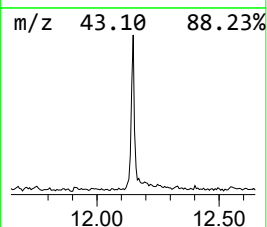
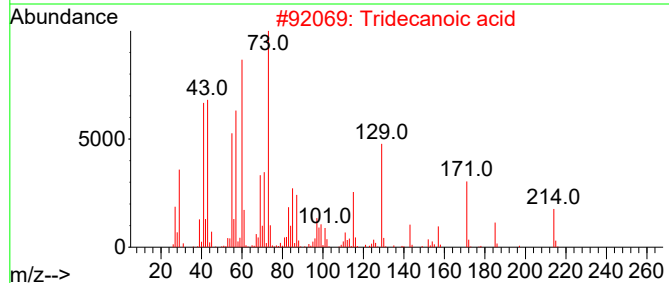
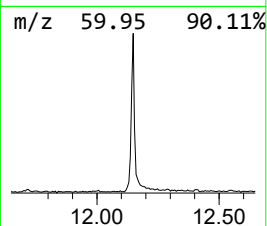
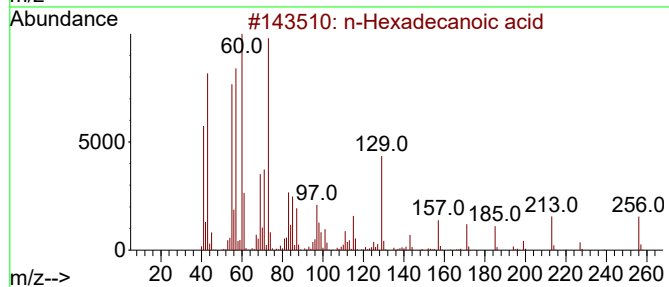
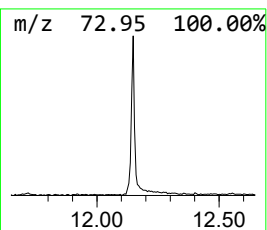
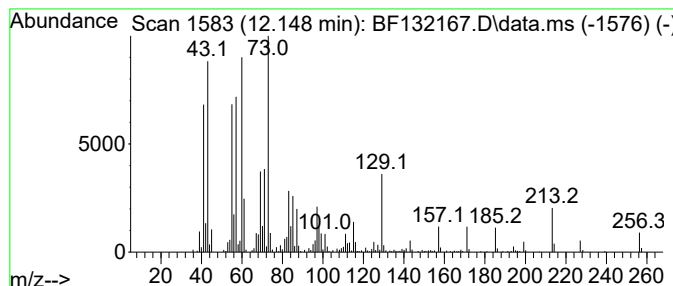
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.148	5.23 ng	428738	Phenanthrene-d10	11.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012023\
Data File : BF132167.D
Acq On : 20 Jan 2023 18:23
Operator : CG\JU
Sample : 01160-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-04-SB02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF011923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.331	26.3	ng	1387730	1	7.089	1055020	20.0
1H-3a,7-Methano...	9.795	7.7	ng	953252	3	10.142	2462460	20.0
Aromadendran ('2')	10.007	5.8	ng	708764	3	10.142	2462460	20.0
Benzene, 1-meth...	10.266	5.0	ng	616563	3	10.142	2462460	20.0
Benzophenone	10.854	3.8	ng	465639	3	10.142	2462460	20.0
n-Hexadecanoic ...	12.148	5.2	ng	428738	4	11.642	1638290	20.0