

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
 Data File : BF124984.D
 Acq On : 7 Aug 2021 20:36
 Operator : JU/CG
 Sample : M3289-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 44043RT

Integration Parameters: rteint.p

Integrator: RTE

Soothing : 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-BF080421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.045	497	503	508	rBB	66627	81283	48.82%	5.420%
2	5.451	568	572	575	rBV	160840	138471	83.18%	9.233%
3	5.669	606	609	616	rBV	6044	8210	4.93%	0.547%
4	5.845	636	639	641	rBB	14467	12403	7.45%	0.827%
5	6.463	739	744	747	rBB	154063	140283	84.26%	9.354%
6	6.828	803	806	809	rBB	46107	32183	19.33%	2.146%
7	7.392	898	902	905	rBB	106788	92422	55.52%	6.162%
8	8.016	1004	1008	1011	rBB	32869	27822	16.71%	1.855%
9	8.110	1021	1024	1027	rBV	59013	44428	26.69%	2.962%
10	9.186	1203	1207	1210	rBB	223255	166479	100.00%	11.100%
11	9.569	1271	1272	1277	rVB3	3514	3294	1.98%	0.220%
12	9.627	1277	1282	1284	rBV4	3471	5769	3.47%	0.385%
13	9.657	1284	1287	1289	rBV3	1516	2233	1.34%	0.149%
14	9.727	1297	1299	1301	rBV	8473	6621	3.98%	0.441%
15	9.774	1304	1307	1309	rVB	10424	8225	4.94%	0.548%
16	9.804	1311	1312	1315	rBV3	2890	3104	1.86%	0.207%
17	9.845	1315	1319	1320	rVV3	5937	6155	3.70%	0.410%
18	9.869	1320	1323	1325	rVB	55327	50359	30.25%	3.358%
19	9.904	1325	1329	1332	rBV3	5015	6783	4.07%	0.452%
20	9.986	1339	1343	1344	rBV3	3549	4368	2.62%	0.291%
21	10.027	1347	1350	1351	rVV3	3589	3405	2.05%	0.227%
22	10.057	1353	1355	1357	rVV3	3431	3271	1.96%	0.218%
23	10.086	1357	1360	1362	rVV3	4727	4714	2.83%	0.314%
24	10.198	1377	1379	1383	rVB5	6127	6179	3.71%	0.412%
25	10.233	1383	1385	1387	rBV3	6711	4997	3.00%	0.333%
26	10.269	1389	1391	1394	rVV3	11546	8709	5.23%	0.581%
27	10.322	1398	1400	1404	rVV4	5969	6637	3.99%	0.443%
28	10.657	1453	1457	1461	rBV	111502	99490	59.76%	6.634%
29	10.780	1476	1478	1481	rVB4	11733	6880	4.13%	0.459%
30	11.357	1573	1576	1578	rBV	59251	48715	29.26%	3.248%
31	12.574	1780	1783	1785	rVB	26215	22476	13.50%	1.499%
32	12.798	1819	1821	1824	rVB	25518	20052	12.04%	1.337%
33	12.939	1842	1845	1850	rVB	143917	145071	87.14%	9.673%
34	13.633	1960	1963	1965	rVB3	5504	4422	2.66%	0.295%
35	13.833	1994	1997	2000	rBV3	12960	13640	8.19%	0.909%
36	13.992	2019	2024	2027	rBV2	45636	54548	32.77%	3.637%

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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

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37	14.015	2027	2028	2031	rVB	14899	10955	6.58%	0.730%
38	14.151	2049	2051	2055	rVB4	3912	3681	2.21%	0.245%
39	14.380	2085	2090	2091	rBV2	2783	3540	2.13%	0.236%
40	14.462	2099	2104	2107	rBV3	5134	7661	4.60%	0.511%
41	14.598	2123	2127	2129	rBV3	1470	2416	1.45%	0.161%
42	14.745	2150	2152	2156	rVB3	1777	2778	1.67%	0.185%
43	14.898	2175	2178	2180	rVB2	4700	3534	2.12%	0.236%
44	15.027	2196	2200	2203	rBV3	18204	24121	14.49%	1.608%
45	15.051	2203	2204	2207	rVV2	8558	5458	3.28%	0.364%
46	15.086	2207	2210	2213	rVV3	7017	7301	4.39%	0.487%
47	15.121	2213	2216	2223	rVB2	7328	12639	7.59%	0.843%
48	15.327	2247	2251	2255	rVB	9423	9794	5.88%	0.653%
49	15.386	2255	2261	2266	rVB	13823	17601	10.57%	1.174%
50	15.451	2266	2272	2275	rBV	27743	33231	19.96%	2.216%
51	15.480	2275	2277	2280	rVB	3000	2465	1.48%	0.164%
52	15.662	2303	2308	2312	rBV	2999	5220	3.14%	0.348%
53	15.886	2342	2346	2351	rBV2	9018	14295	8.59%	0.953%
54	15.951	2353	2357	2360	rVB3	1974	3279	1.97%	0.219%
55	16.380	2425	2430	2431	rBV3	2024	2637	1.58%	0.176%
56	16.674	2476	2480	2484	rBB2	3107	4535	2.72%	0.302%
57	16.898	2513	2518	2525	rBV2	5104	8583	5.16%	0.572%
58	16.974	2525	2531	2534	rVB2	2214	4462	2.68%	0.298%
59	17.074	2545	2548	2554	rVB2	1738	2683	1.61%	0.179%
60	17.221	2569	2573	2577	rVB2	2717	3686	2.21%	0.246%
61	17.345	2589	2594	2599	rVB2	3973	5861	3.52%	0.391%
62	17.480	2613	2617	2624	rVB3	1910	3232	1.94%	0.216%

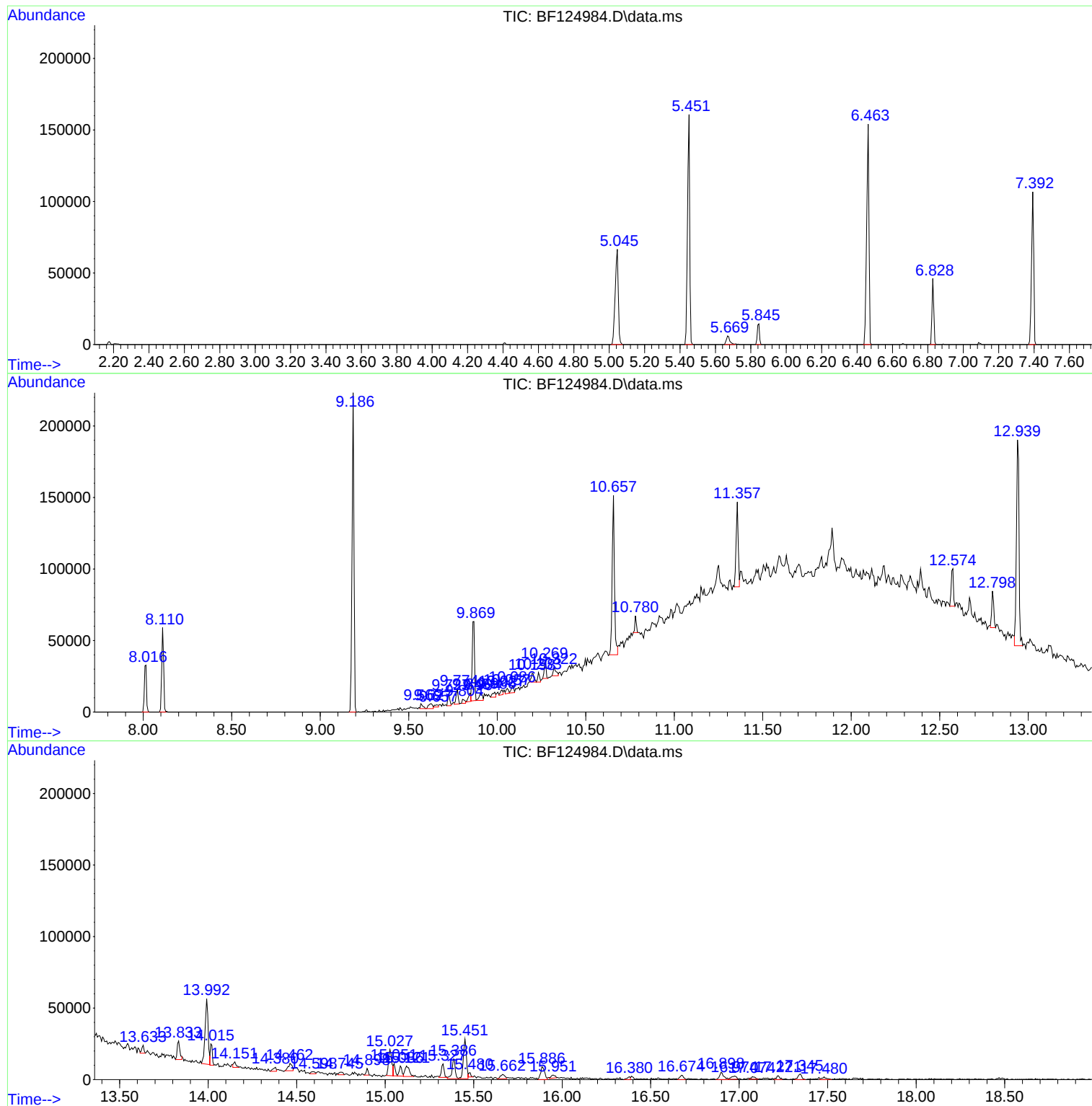
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : M3289-05
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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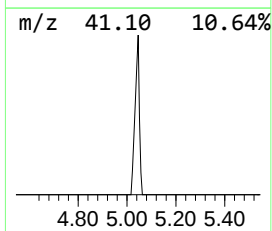
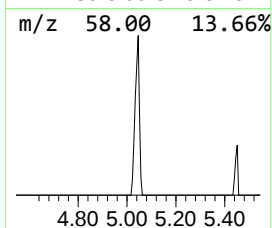
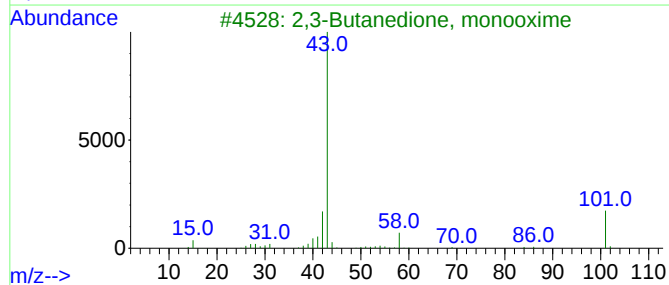
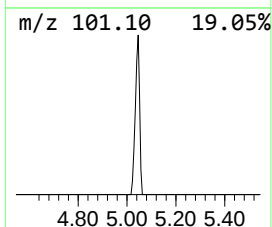
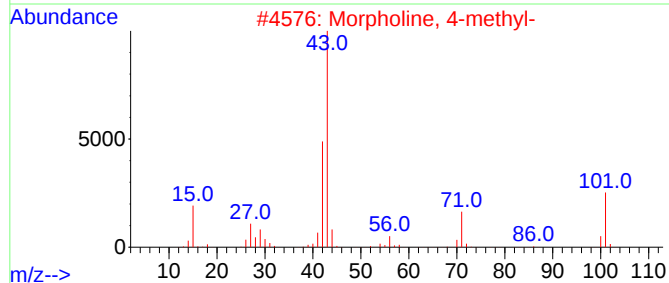
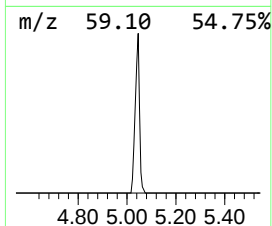
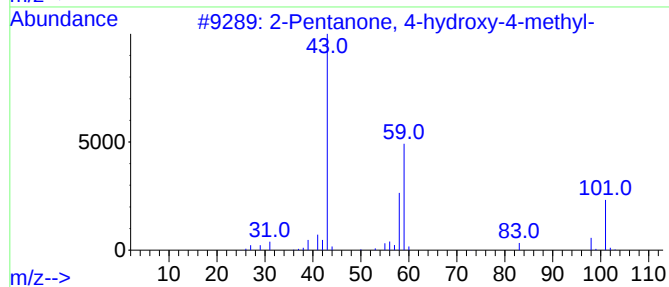
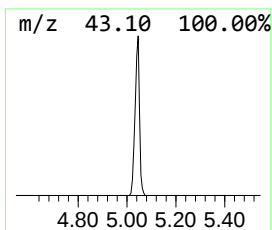
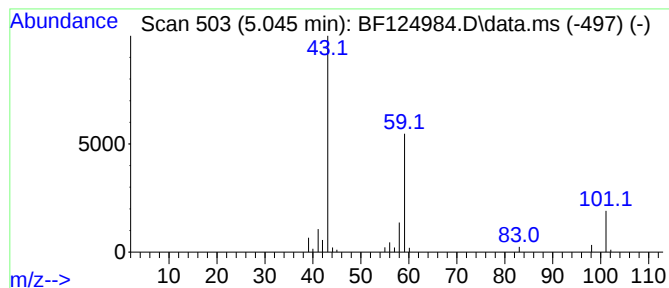
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	50.51 ng	81283	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	9		
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9		



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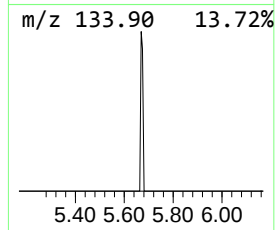
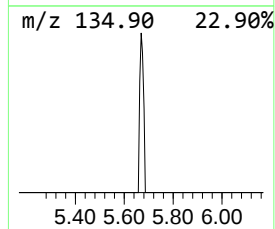
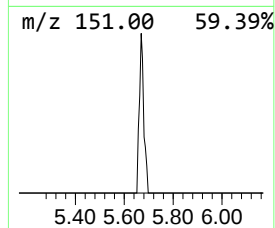
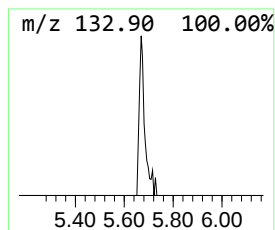
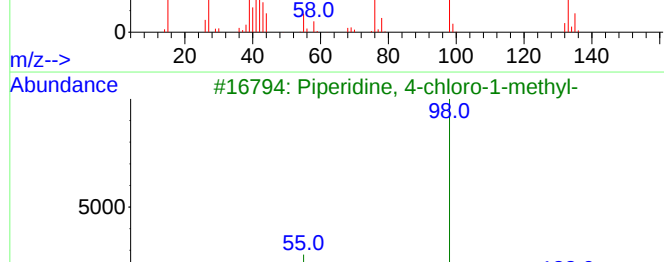
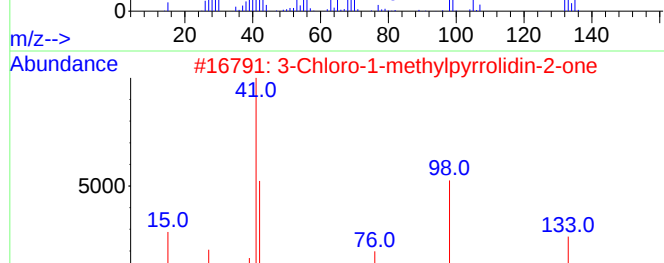
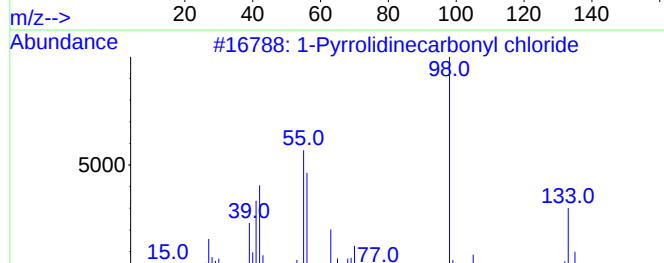
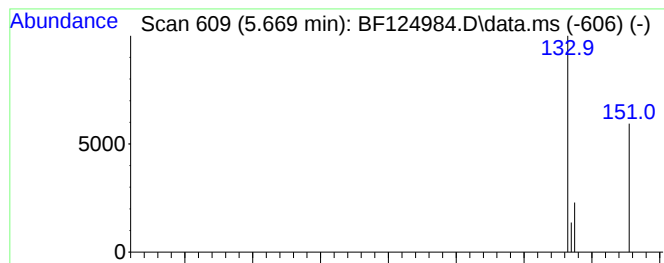
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.669 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.669	5.10 ng	8210	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pyrrolidinecarbonyl chloride	133	C5H8ClNO	001192-63-8	7
2			3-Chloro-1-methylpyrrolidin-2-one	133	C5H8ClNO	1000487-04-2	5
3			Piperidine, 4-chloro-1-methyl-	133	C6H12ClN	005570-77-4	5
4			N-Chlorosuccinimide	133	C4H4ClNO2	000128-09-6	5
5			(5-Chloro-1H-1,2,4-triazol-3-yl)...	133	C3H4ClN3O	1000387-64-6	5



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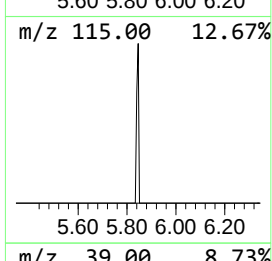
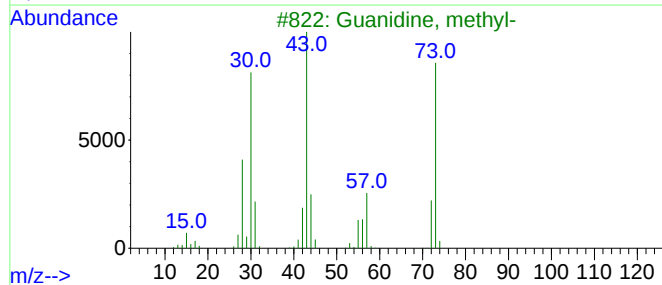
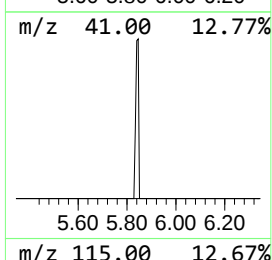
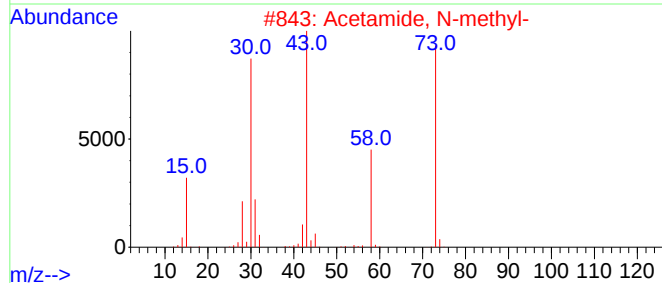
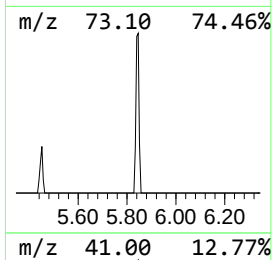
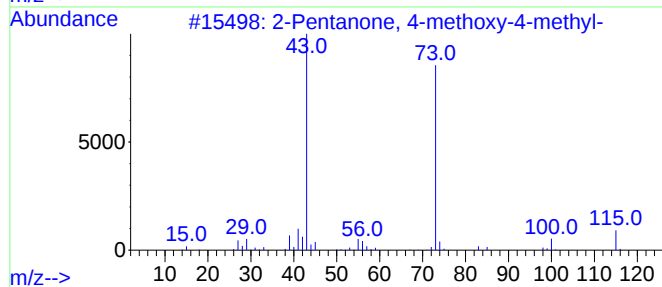
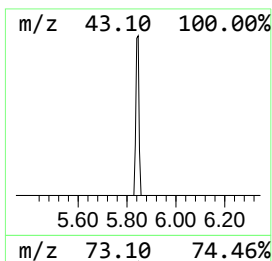
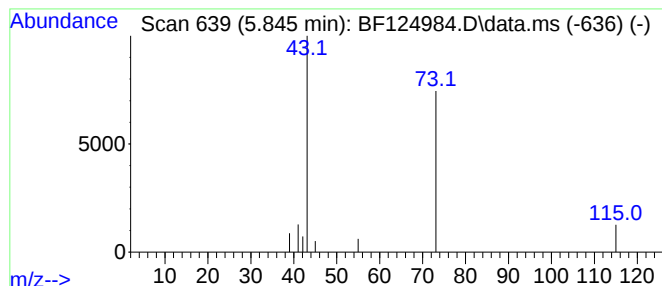
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.845	7.71 ng	12403	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	64		
2	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9		
3	Guanidine, methyl-	73	C2H7N3	000471-29-4	5		
4	N-Ethylformamide	73	C3H7NO	000627-45-2	5		
5	Acetamide, N-(2-methylpropyl)-	115	C6H13NO	001540-94-9	4		



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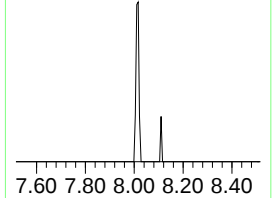
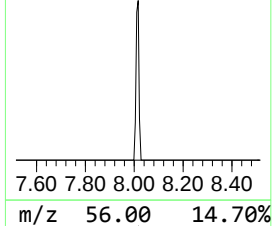
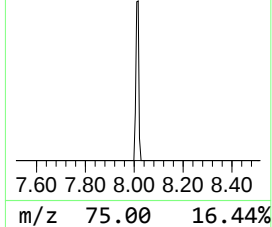
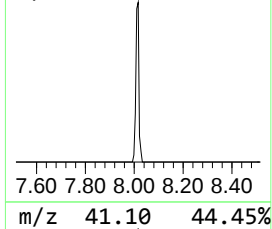
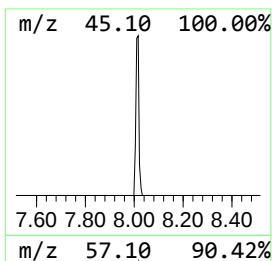
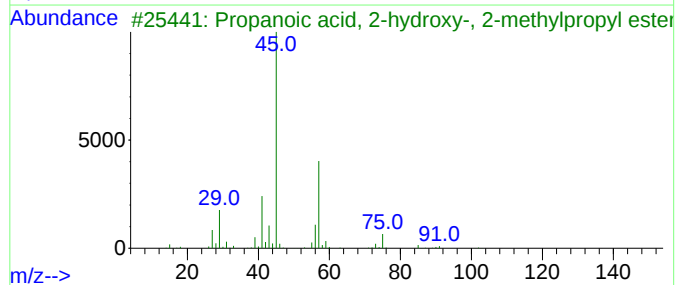
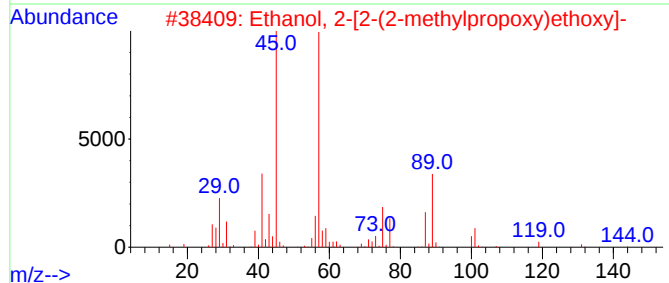
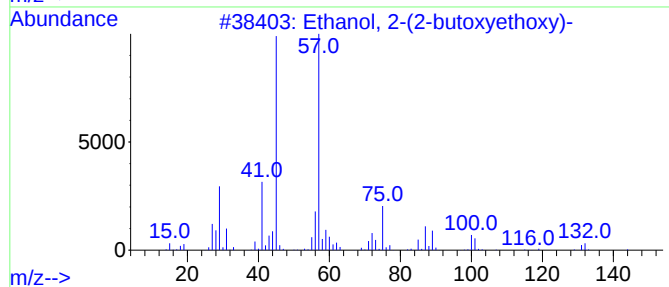
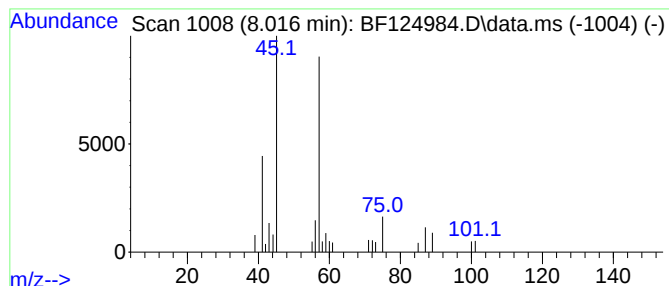
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.016	12.52 ng	27822	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)ethoxy]-	162	C8H18O3	018912-80-6	64
3			Propanoic acid, 2-hydroxy-, 2-methylpropyl ester	146	C7H14O3	000585-24-0	53
4			Ethanol, 2-[2-(2-butoxyethoxy)ethoxy]-	206	C10H22O4	000143-22-6	37
5			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	36



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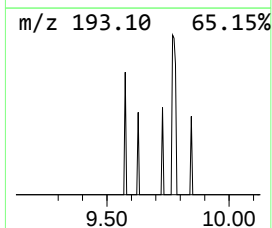
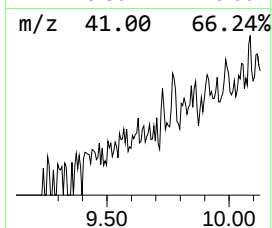
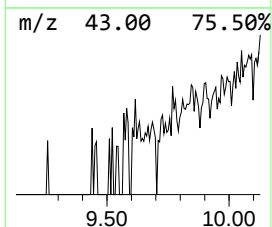
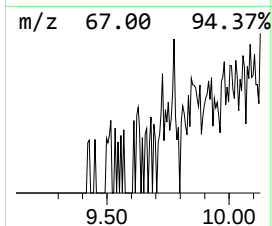
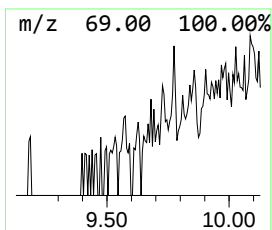
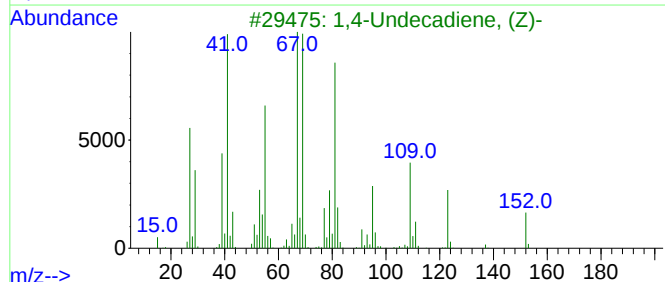
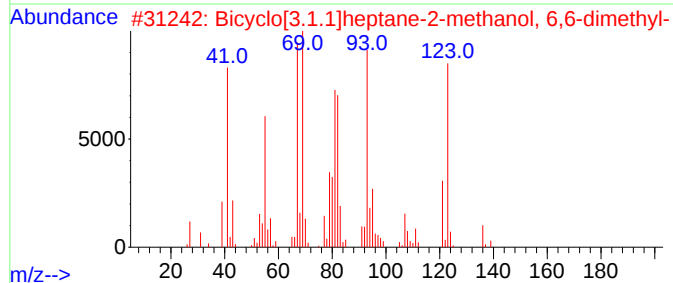
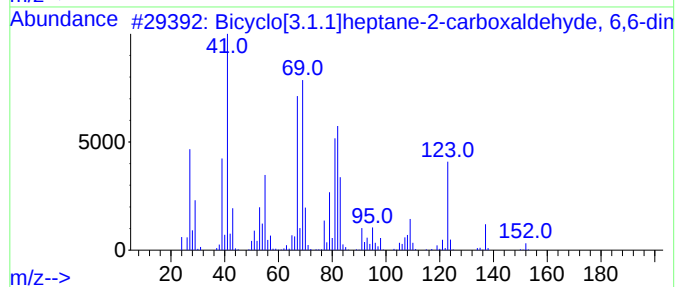
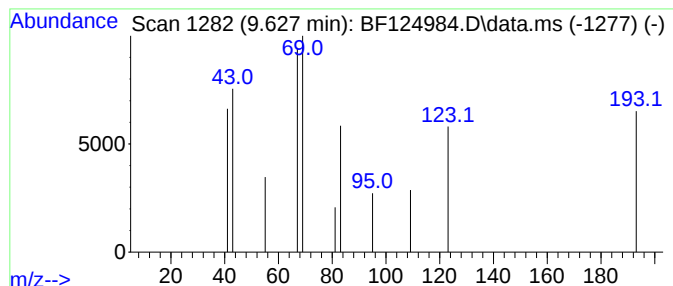
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Bicyclo[3.1.1]heptane-2-car... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.627	2.29 ng	5769	Acenaphthene-d10	9.869	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptane-2-carboxal...	152	C10H16O	004764-14-1	64
2	Bicyclo[3.1.1]heptane-2-methanol...	154	C10H18O	000514-99-8	36
3	1,4-Undecadiene, (Z)-	152	C11H20	055976-14-2	33
4	(-)-cis-Myrtanol	154	C10H18O	051152-12-6	33
5	Propane, 2-(2-isopropylidene-3-m...	138	C10H18	024524-51-4	23



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
Operator : JU/CG
Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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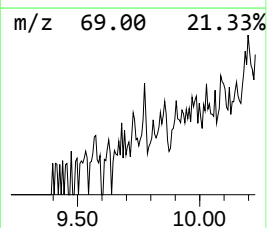
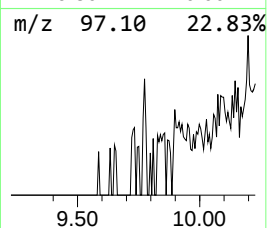
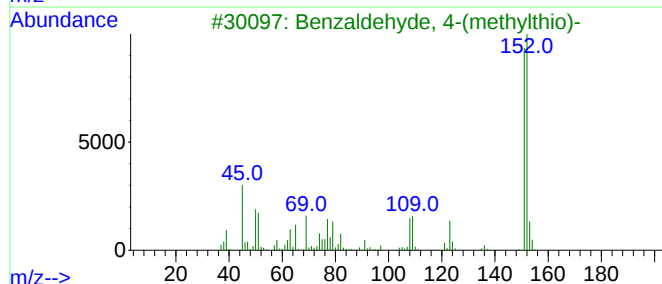
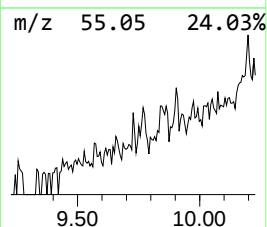
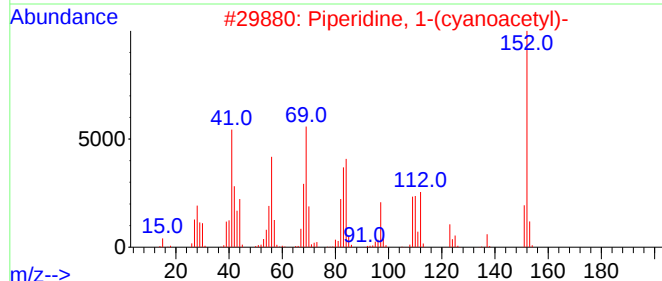
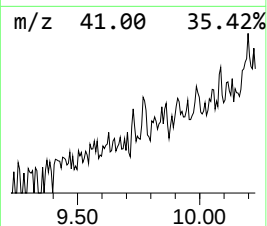
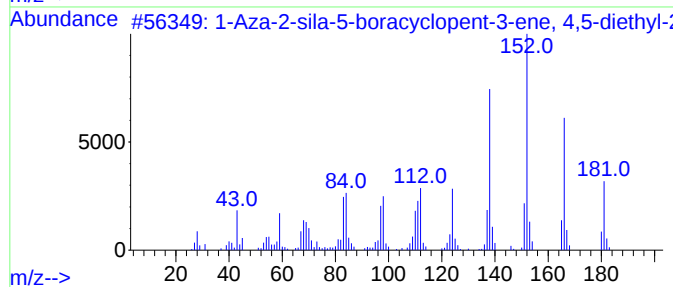
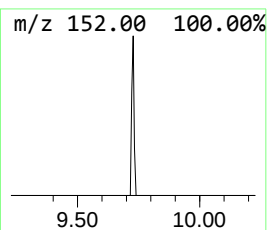
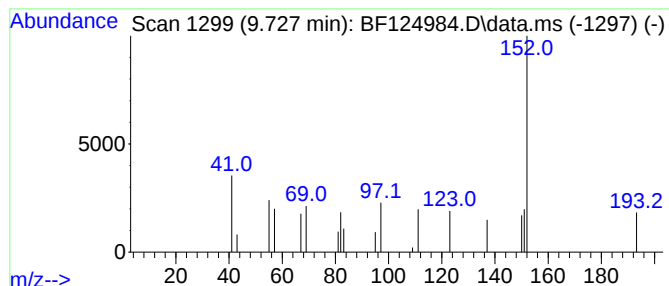
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Aza-2-sila-5-boracyclopent... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.727	2.63 ng	6621	Acenaphthene-d10	9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Aza-2-sila-5-boracyclopent-3-e...	181	C9H20BNSi	107098-32-8	59
2		Piperidine, 1-(cyanoacetyl)-	152	C8H12N2O	015029-30-8	47
3		Benzaldehyde, 4-(methylthio)-	152	C8H8OS	003446-89-7	9
4		Benzaldehyde, 2-hydroxy-5-methoxy-	152	C8H8O3	000672-13-9	9
5		5,6-Dihydro-4-methylthieno(2,3-d...	152	C7H8N2S	092204-06-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
Operator : JU/CG
Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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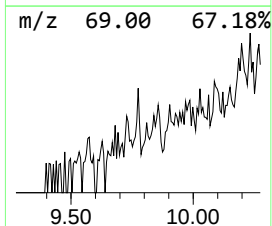
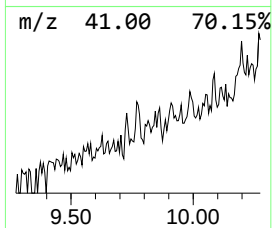
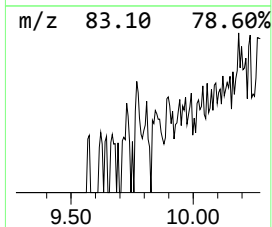
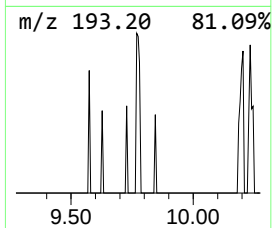
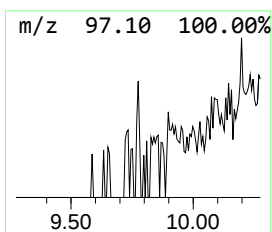
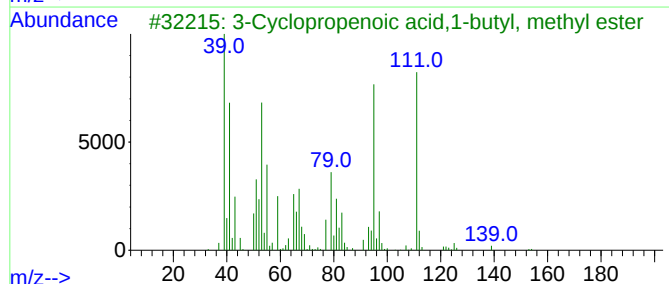
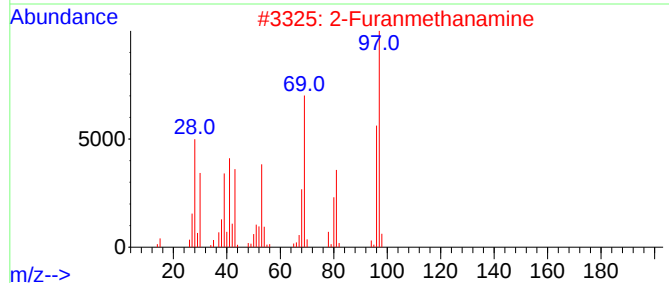
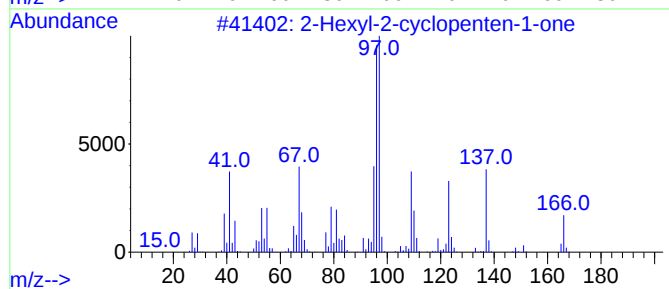
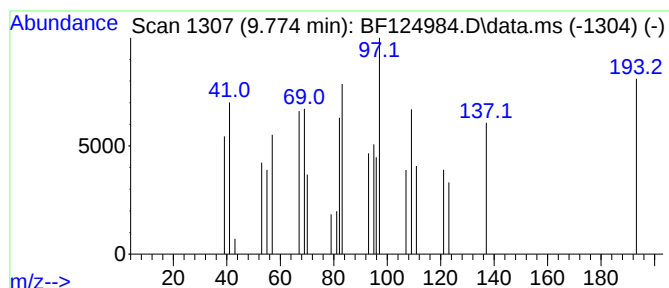
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown9.774 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.774	3.27 ng	8225	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexyl-2-cyclopenten-1-one	166	C11H18O	000095-41-0	38		
2	2-Furanmethanamine	97	C5H7NO	000617-89-0	27		
3	3-Cyclopropenoic acid,1-butyl, m...	154	C9H14O2	067500-40-7	22		
4	Cyclopentaneacetaldehyde, 2-form...	166	C10H14O2	005951-57-5	22		
5	cis-p-mentha-1(7),8-dien-2-ol	152	C10H16O	1000374-16-8	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
Operator : JU/CG
Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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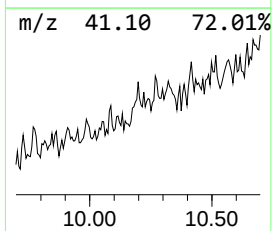
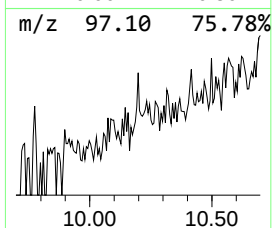
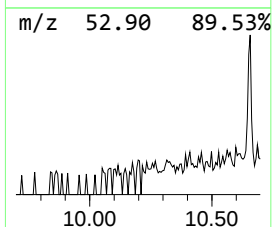
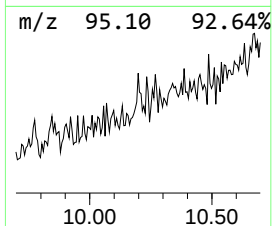
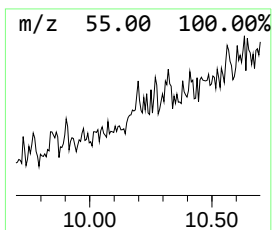
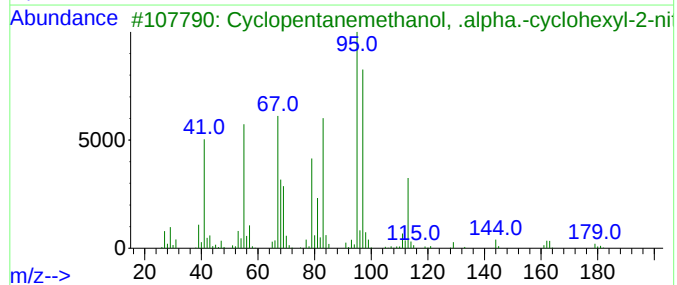
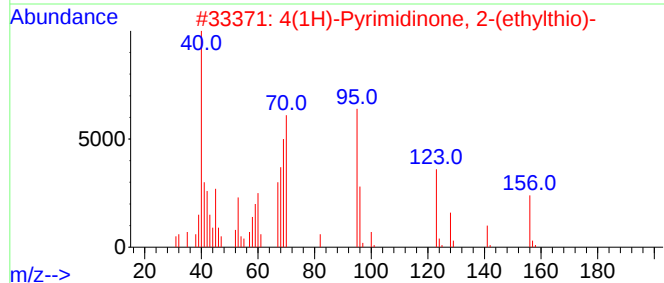
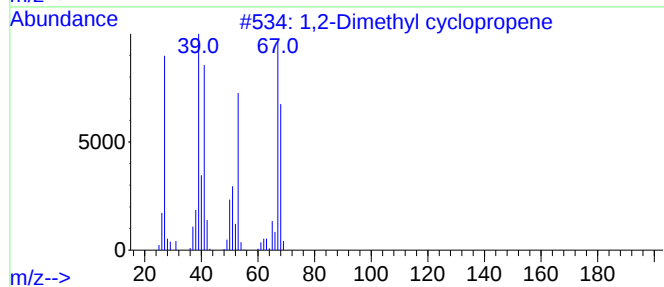
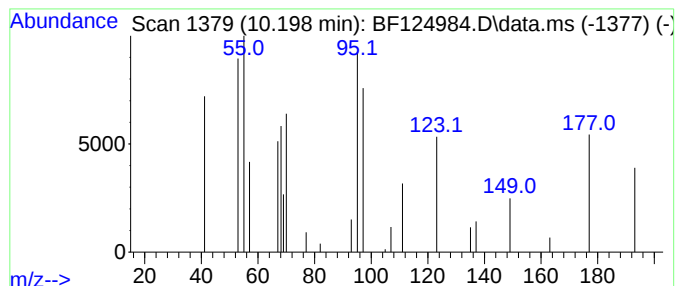
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.198 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	2.45 ng	6179	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dimethyl cyclopropene	68	C5H8	014309-32-1	9
2			4(1H)-Pyrimidinone, 2-(ethylthio)-	156	C6H8N2OS	006965-19-1	9
3			Cyclopentanemethanol, .alpha.-cy...	227	C12H21NO3	103077-58-3	9
4			2-Furanmethanol	98	C5H6O2	000098-00-0	9
5			Cyclopentaneacetaldehyde, 2-form...	166	C10H14O2	005951-57-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
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Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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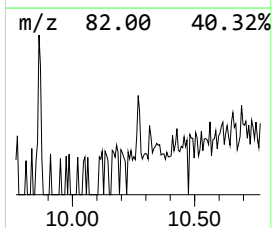
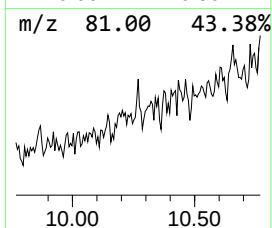
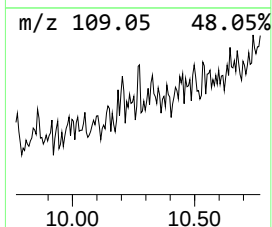
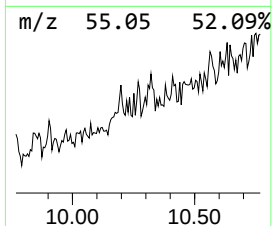
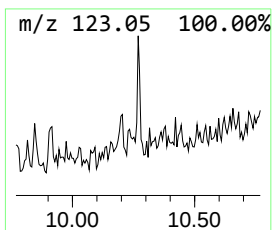
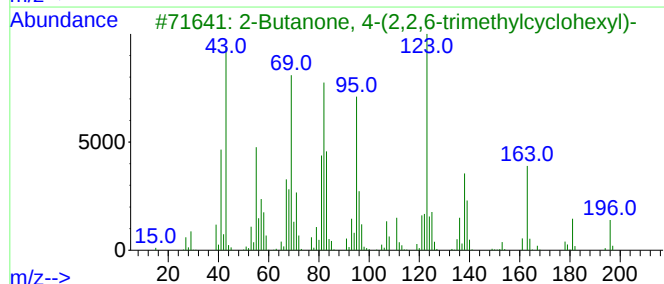
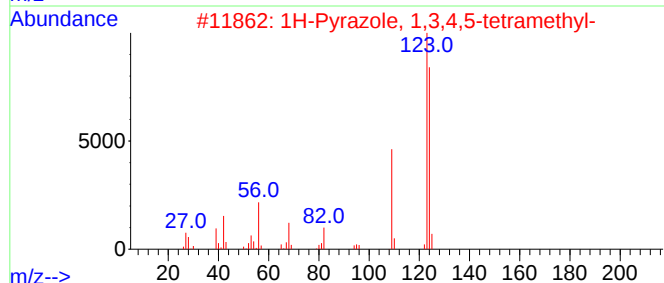
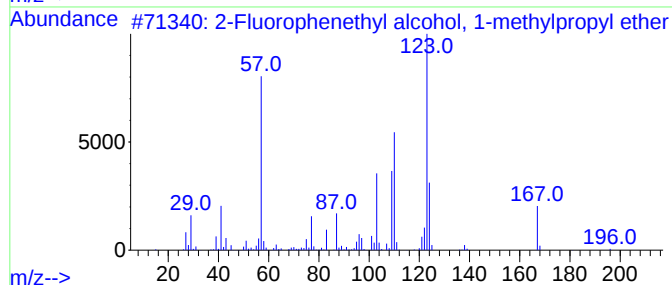
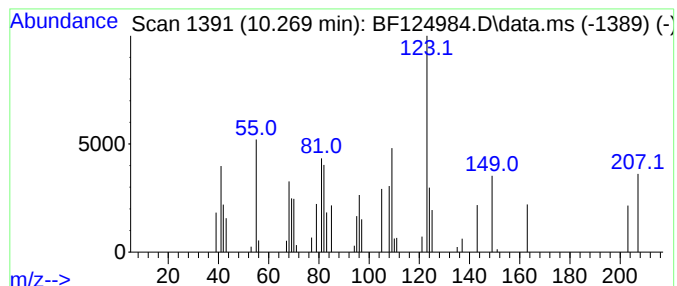
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.269 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.269	3.46 ng	8709	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Fluorophenethyl alcohol, 1-met...	196	C12H17FO	1000394-96-5	23		
2	1H-Pyrazole, 1,3,4,5-tetramethyl-	124	C7H12N2	001073-20-7	17		
3	2-Butanone, 4-(2,2,6-trimethylcy...	196	C13H24O	006138-85-8	13		
4	Cyclohexanol, 3-(aminomethyl)-3,...	171	C10H21NO	015647-11-7	12		
5	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	12		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
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Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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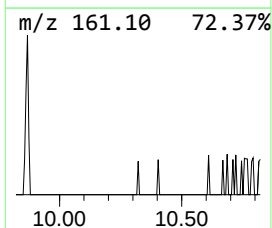
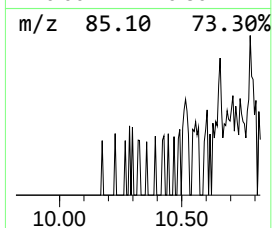
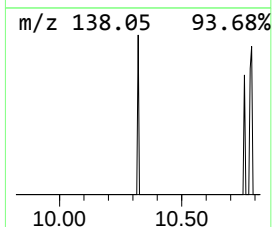
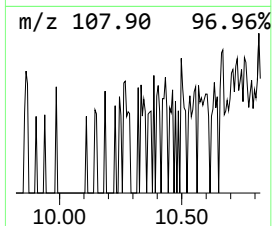
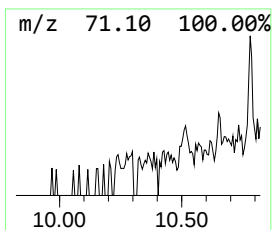
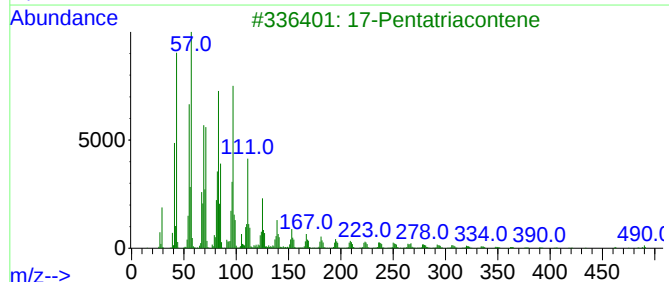
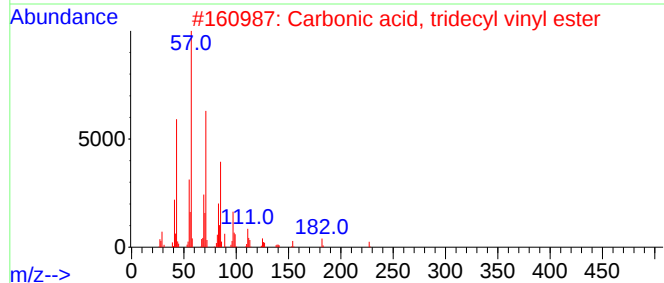
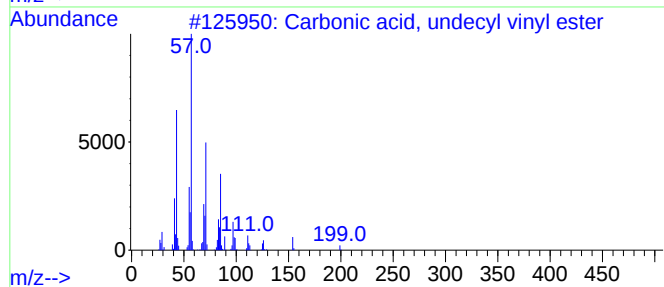
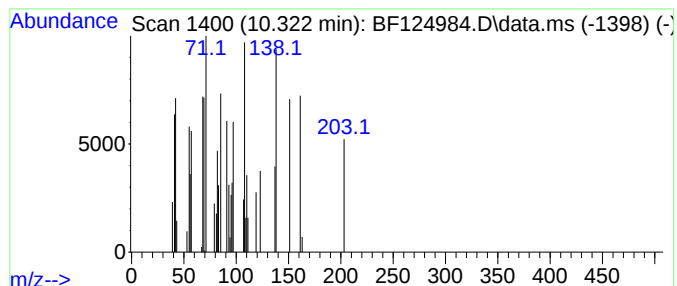
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.322 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.322	2.64 ng	6637	Acenaphthene-d10	9.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, undecyl vinyl ester	242	C14H26O3	1000382-54-9	14
2			Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	14
3			17-Pentatriacontene	491	C35H70	006971-40-0	14
4			Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	12
5			Docosyl isobutyl ether	382	C26H54O	1000406-33-1	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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ALS Vial : 11 Sample Multiplier: 1

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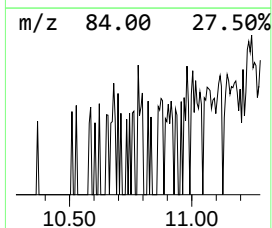
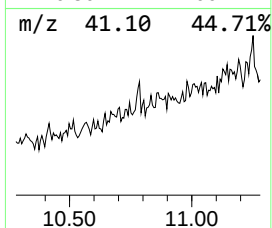
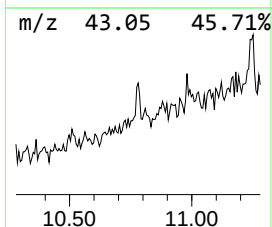
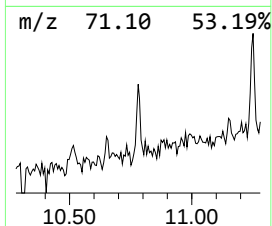
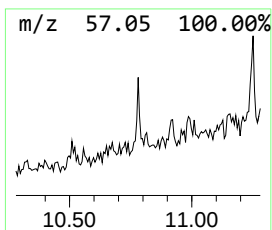
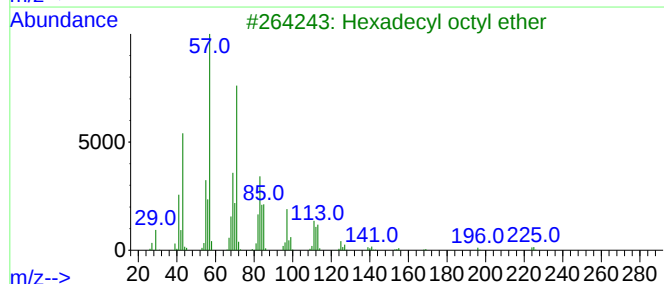
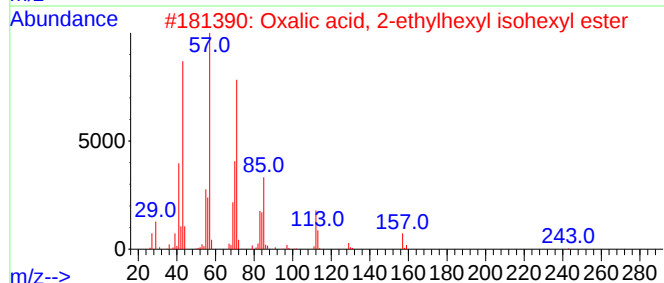
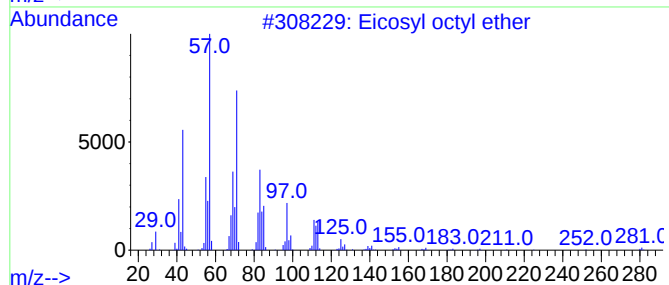
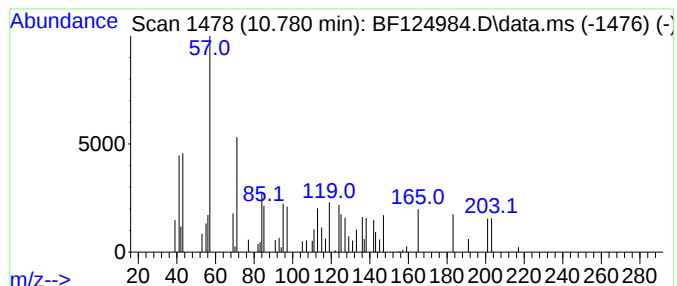
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown10.780 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.780	2.82 ng	6880	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosyl octyl ether	410	C28H58O	1000406-38-8	25
2			Oxalic acid, 2-ethylhexyl isohex...	286	C16H30O4	1000309-38-8	22
3			Hexadecyl octyl ether	354	C24H50O	1000406-38-6	16
4			Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	16
5			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
Operator : JU/CG
Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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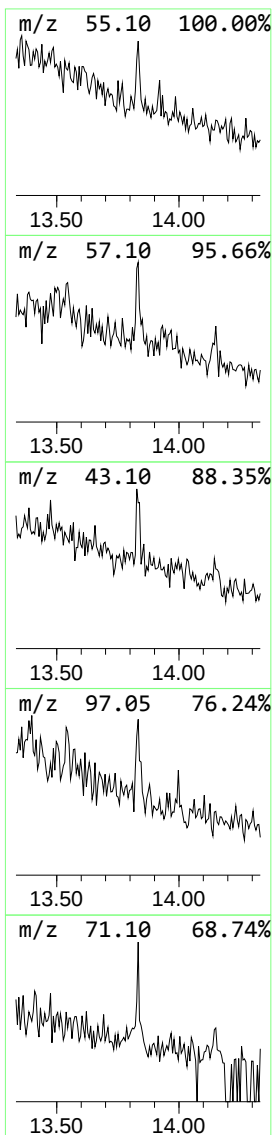
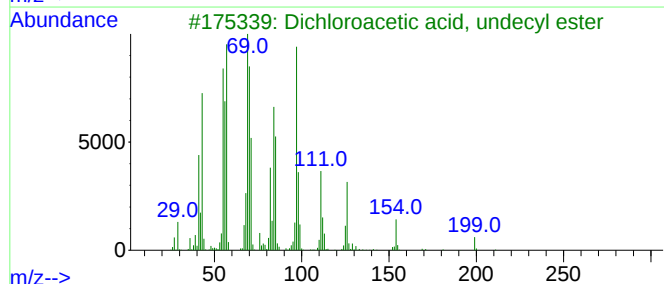
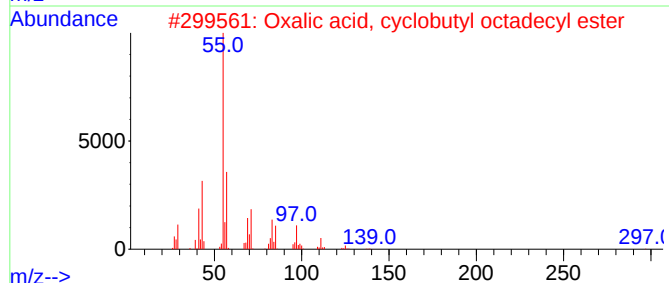
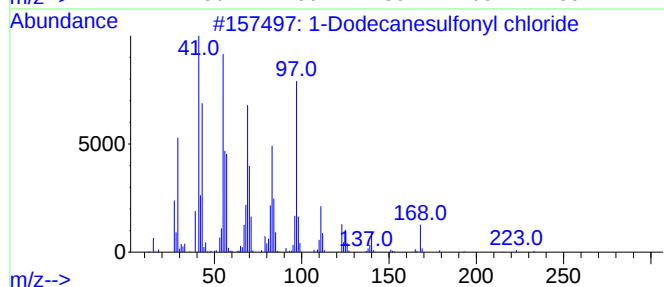
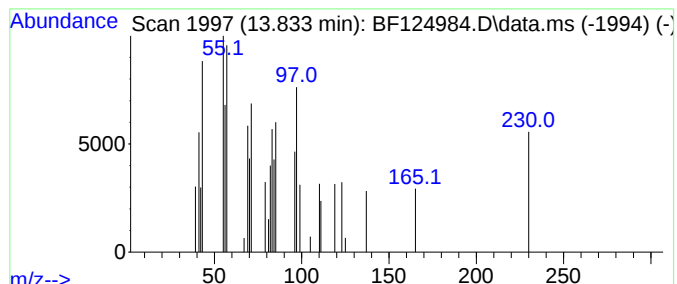
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown13.833 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	5.00 ng	13640	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanesulfonyl chloride	268	C12H25ClO2S	010147-40-7	27
2			Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	22
3			Dichloroacetic acid, undecyl ester	282	C13H24Cl2O2	090146-85-3	22
4			1,10-Dicyanodecane	192	C12H20N2	004543-66-2	22
5			1-Octanol, 2-butyl-	186	C12H26O	003913-02-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
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Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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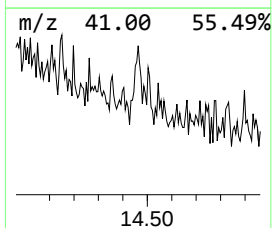
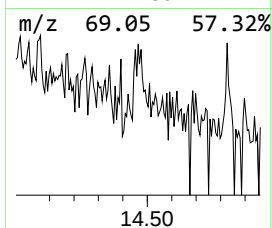
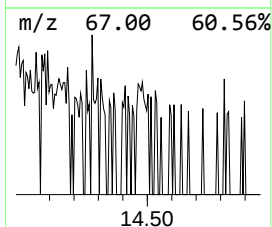
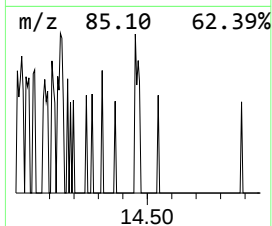
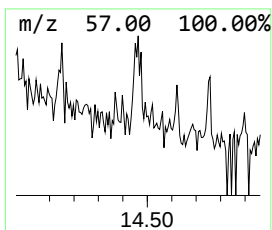
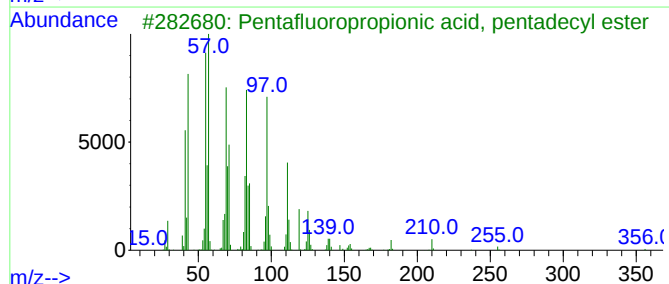
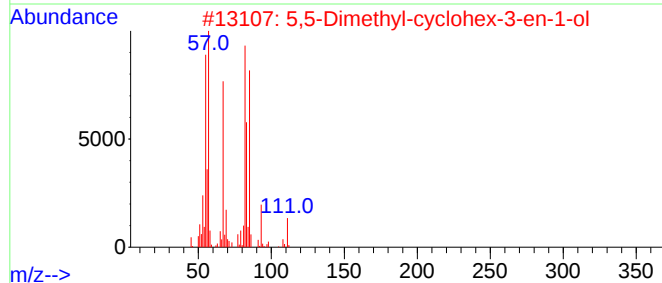
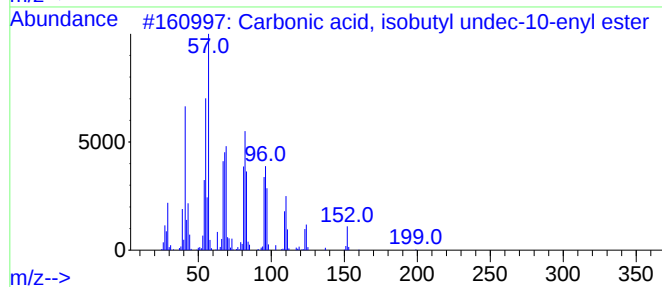
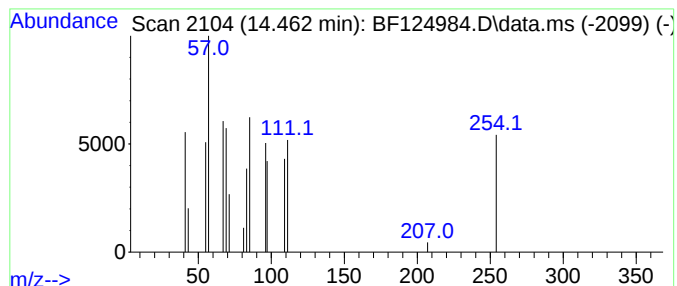
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown14.462 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.462	2.81 ng	7661	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, isobutyl undec-10...	270	C16H30O3	1000314-60-8	37
2			5,5-Dimethyl-cyclohex-3-en-1-ol	126	C8H14O	082299-68-1	35
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	27
4			3-Octadecene, (E)-	252	C18H36	007206-19-1	27
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
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Sample : M3289-05
Misc :
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ClientSampleId :
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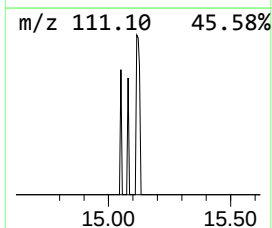
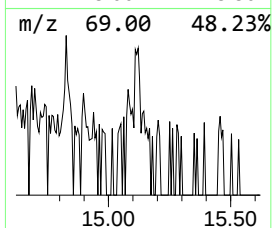
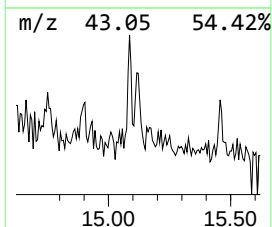
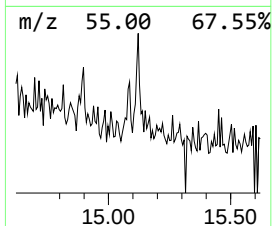
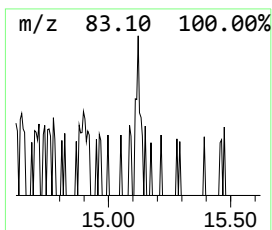
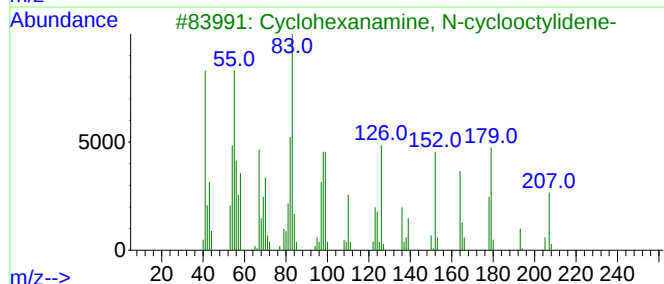
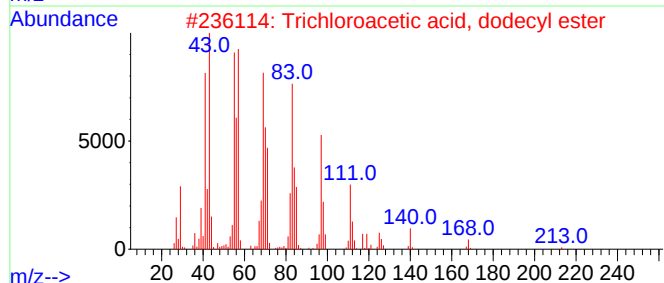
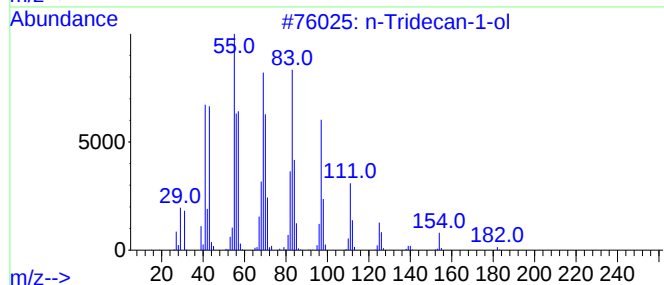
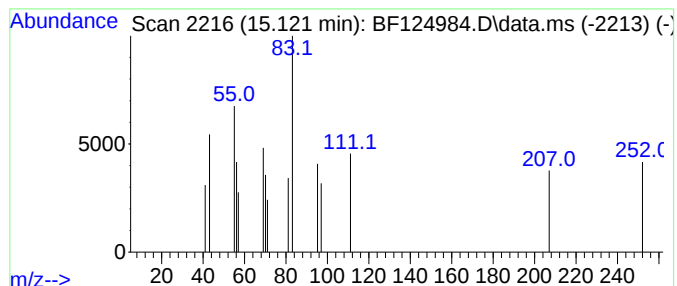
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown15.121 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.121	7.61 ng	12639	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tridecan-1-ol	200	C13H28O	000112-70-9	35
2			Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	35
3			Cyclohexanamine, N-cyclooctylidene-	207	C14H25N	054699-42-2	35
4			Cyclohexadecane	224	C16H32	000295-65-8	35
5			Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
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Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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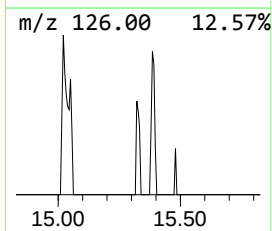
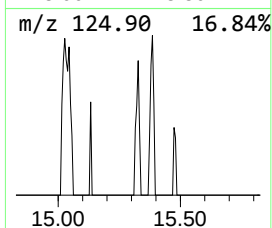
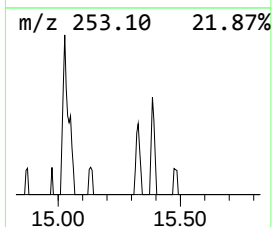
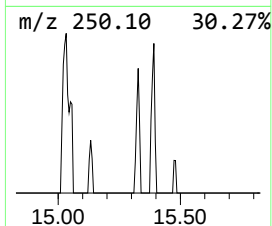
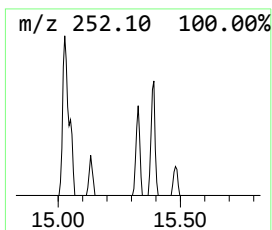
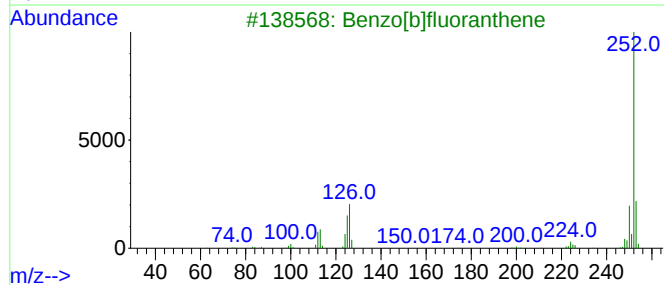
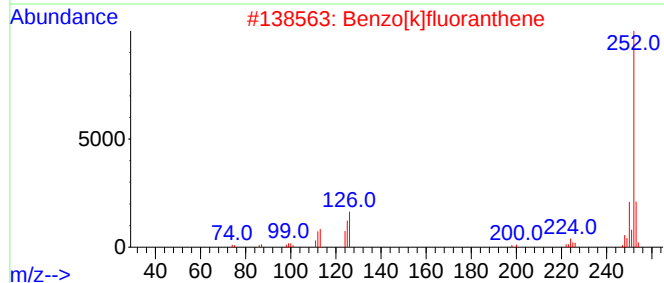
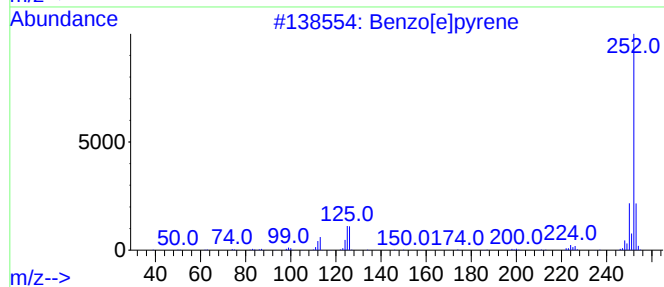
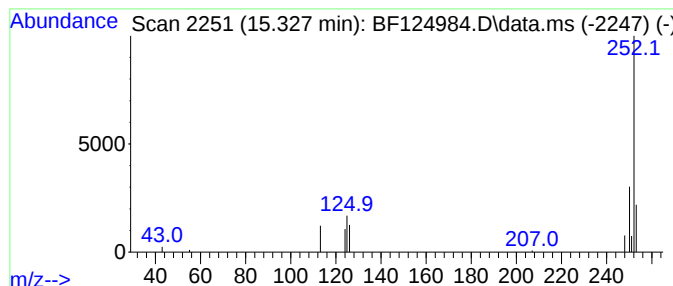
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.327	5.89 ng	9794	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	80
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	80
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	72
4			Perylene	252	C20H12	000198-55-0	72
5			Benzo[a]pyrene	252	C20H12	000050-32-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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Acq On : 7 Aug 2021 20:36
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Sample : M3289-05
Misc :
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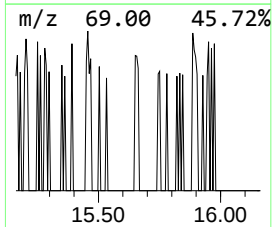
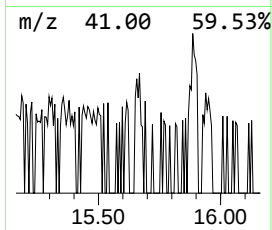
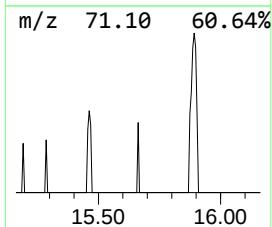
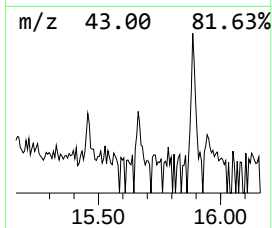
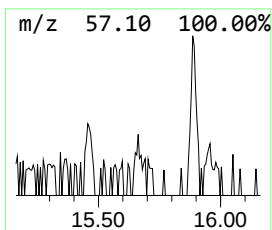
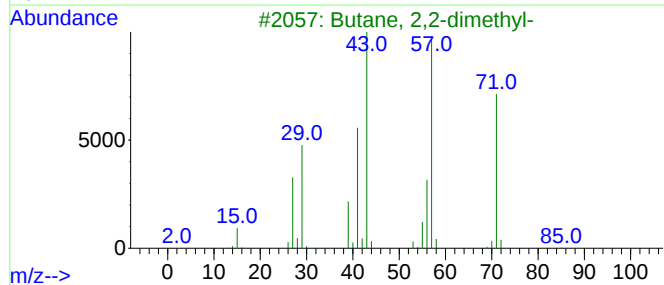
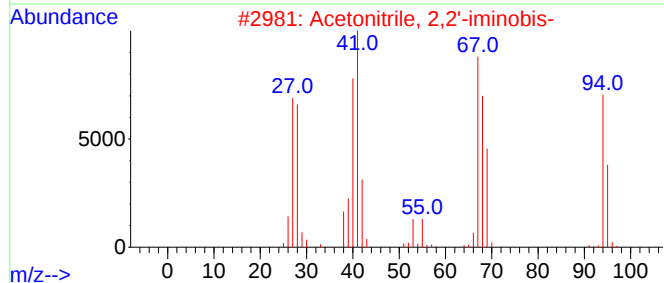
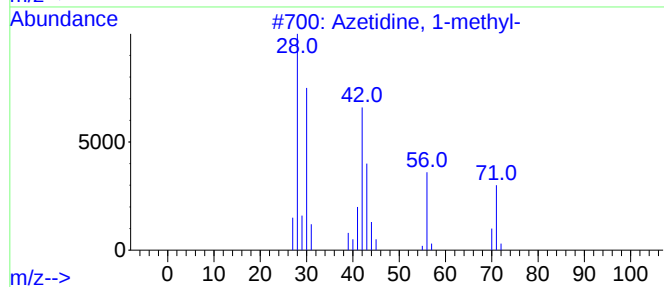
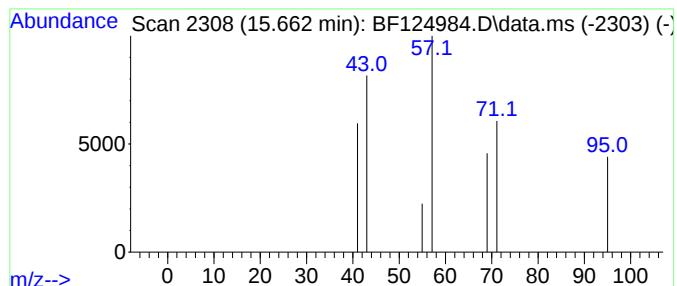
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown15.662 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.662	3.14 ng	5220	Perylene-d12	15.451	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
2	Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	4
3	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4
4	Hexanal, 5,5-dimethyl-	128	C8H16O	055320-58-6	4
5	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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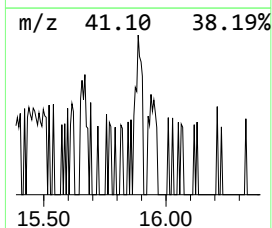
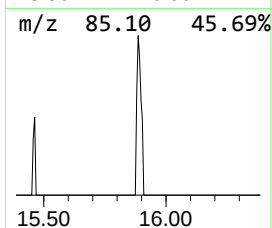
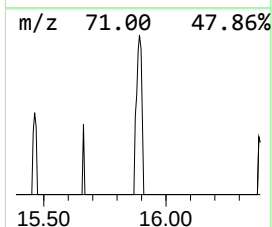
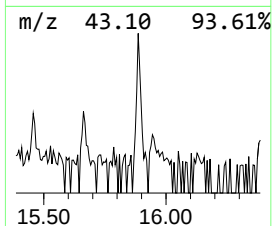
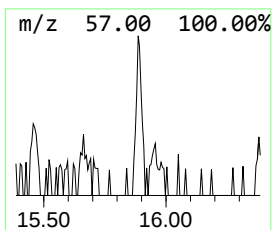
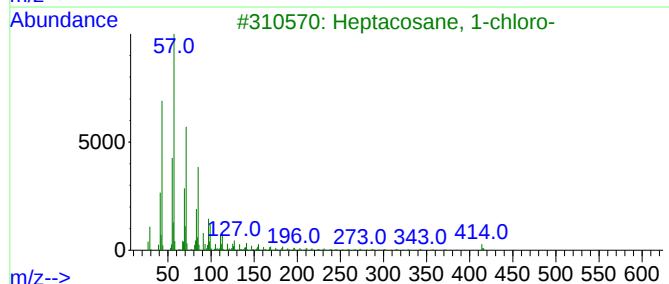
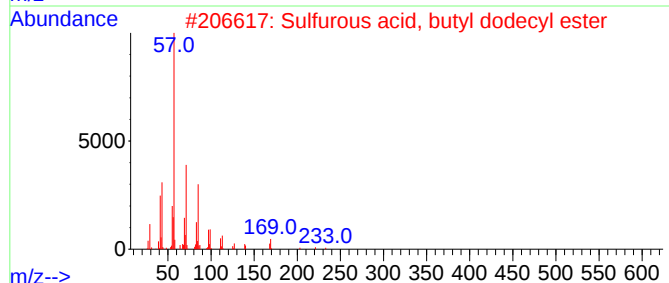
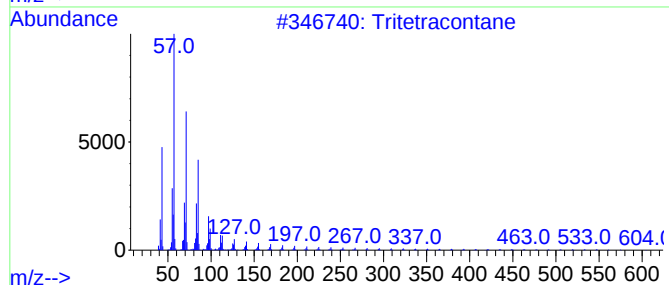
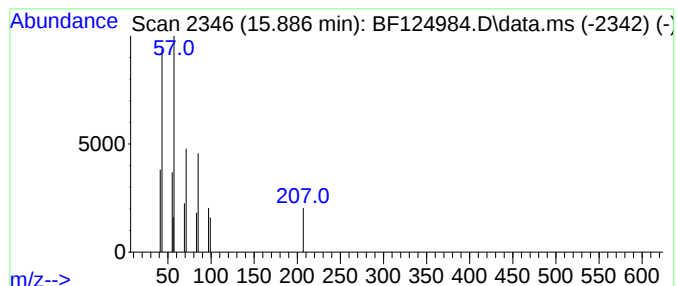
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Tritetracontane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	8.60 ng	14295	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	64
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	64
3			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	64
4			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	64
5			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
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Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

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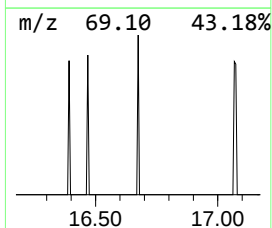
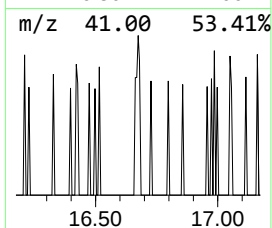
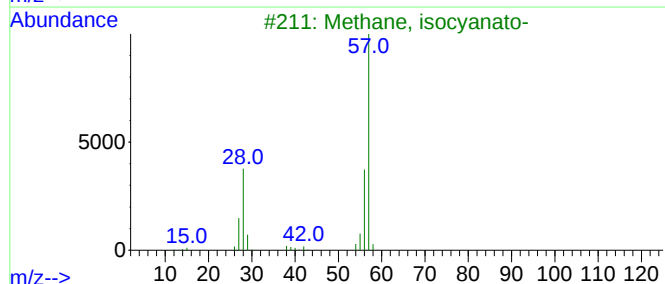
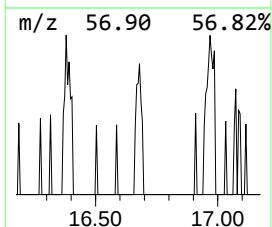
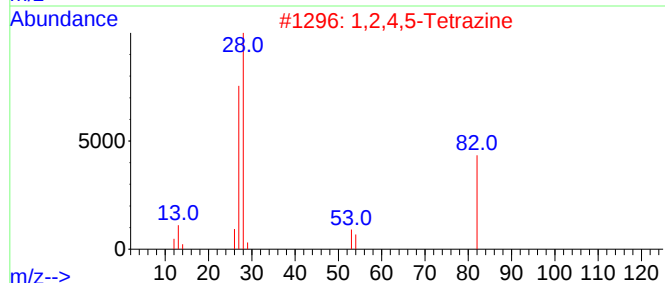
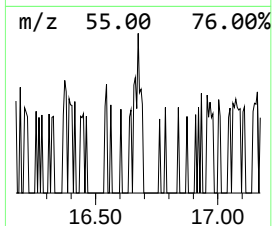
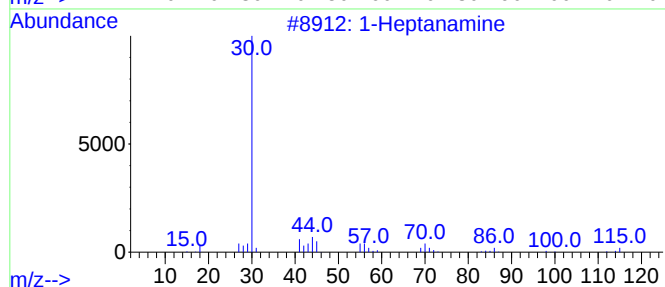
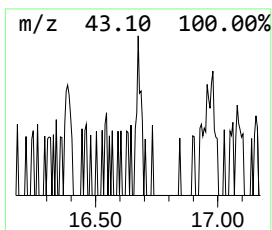
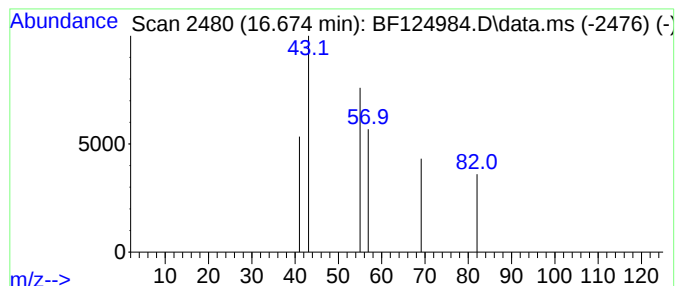
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown16.674 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.674	2.73 ng	4535	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptanamine	115	C7H17N	000111-68-2	2
2			1,2,4,5-Tetrazine	82	C2H2N4	000290-96-0	2
3			Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4			1,4-Pentadien-3-one	82	C5H6O	001890-28-4	1
5			Ethyl isocyanide	55	C3H5N	000624-79-3	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
Operator : JU/CG
Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
44043RT

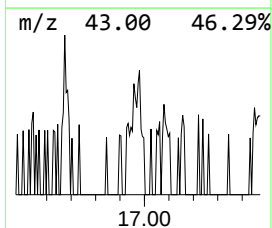
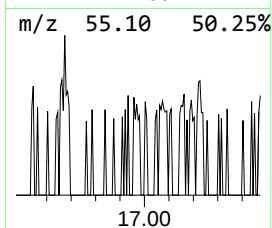
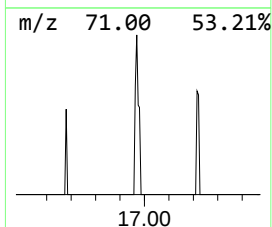
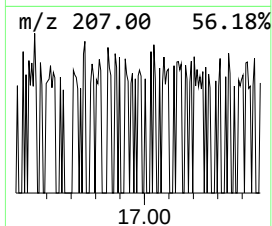
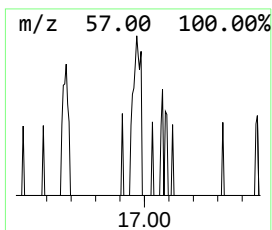
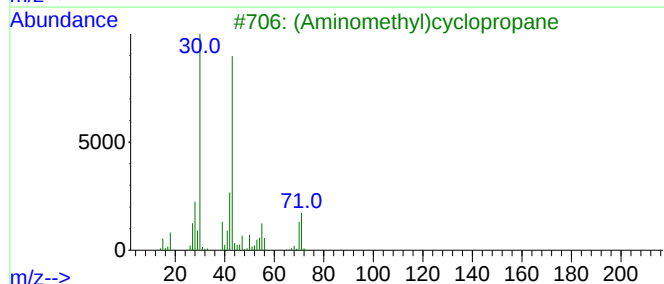
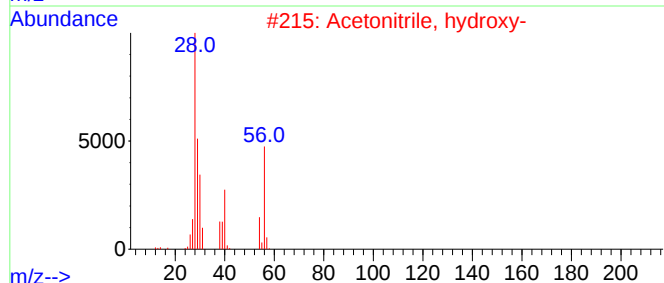
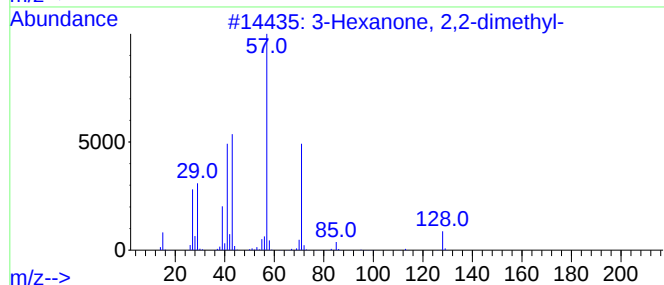
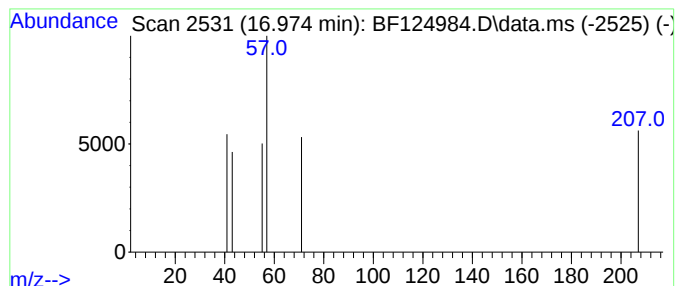
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown16.974 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD		R.T.
16.974	2.69 ng	4462	Perylene-d12		15.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2,2-dimethyl-	128	C8H16O	005405-79-8	4	
2	Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3	
3	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3	
4	1-Pentanol, 4-methyl-2-methylene-	114	C7H14O	121505-31-5	2	
5	Heptane, 3-(bromomethyl)-	192	C8H17Br	018908-66-2	2	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
Operator : JU/CG
Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
44043RT

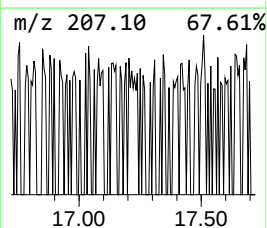
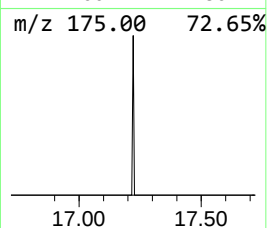
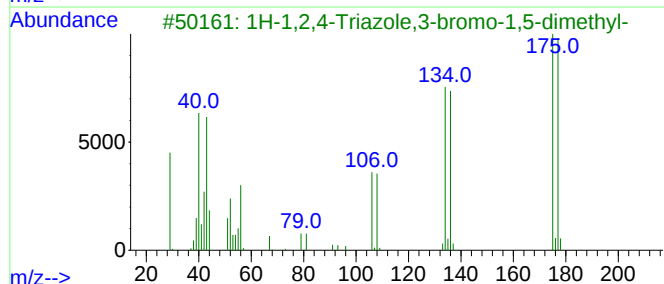
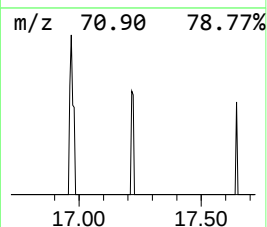
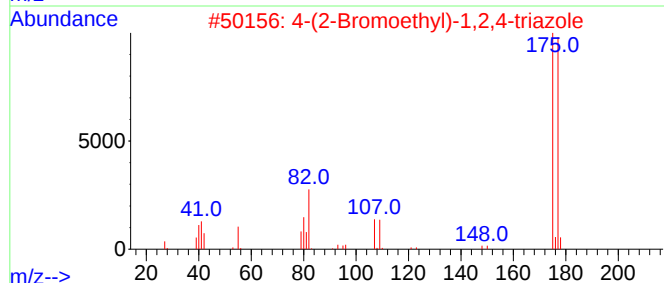
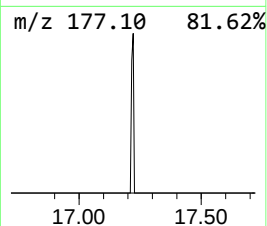
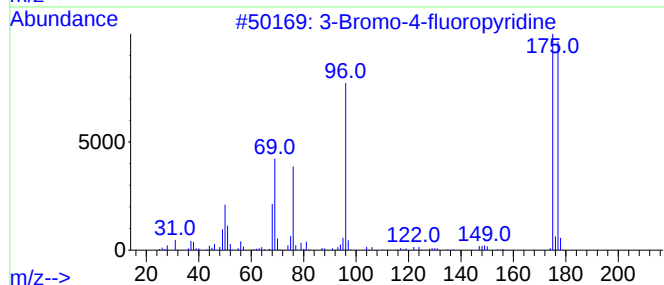
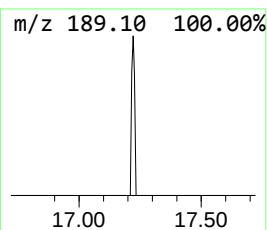
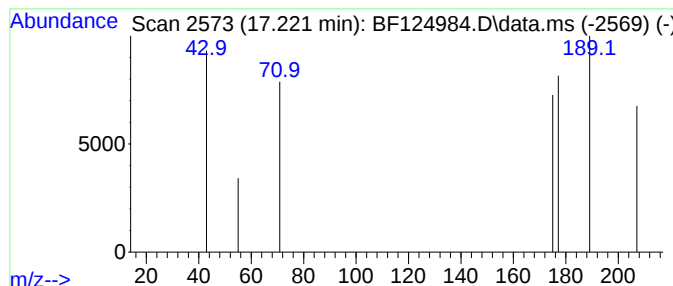
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown17.221 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.221	2.22 ng	3686	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Bromo-4-fluoropyridine	175	C5H3BrFN	116922-60-2	5
2			4-(2-Bromoethyl)-1,2,4-triazole	175	C4H6BrN3	1000459-77-6	5
3			1H-1,2,4-Triazole,3-bromo-1,5-di...	175	C4H6BrN3	056616-93-4	5
4			3-Bromo-2-fluoropyridine	175	C5H3BrFN	036178-05-9	5
5			1H-Pyrazole, 3-amino-4-bromo-5-m...	175	C4H6BrN3	1000302-53-9	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124984.D
Acq On : 7 Aug 2021 20:36
Operator : JU/CG
Sample : M3289-05
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
44043RT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.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-...	5.045	50.5	ng	81283	1	6.828	32183	20.0
unknown5.669	5.669	5.1	ng	8210	1	6.828	32183	20.0
2-Pentanone, 4-...	5.845	7.7	ng	12403	1	6.828	32183	20.0
Ethanol, 2-(2-b...	8.016	12.5	ng	27822	2	8.110	44428	20.0
Bicyclo[3.1.1]h...	9.627	2.3	ng	5769	3	9.869	50359	20.0
1-Aza-2-sila-5-...	9.727	2.6	ng	6621	3	9.869	50359	20.0
unknown9.774	9.774	3.3	ng	8225	3	9.869	50359	20.0
unknown10.198	10.198	2.5	ng	6179	3	9.869	50359	20.0
unknown10.269	10.269	3.5	ng	8709	3	9.869	50359	20.0
unknown10.322	10.322	2.6	ng	6637	3	9.869	50359	20.0
unknown10.780	10.780	2.8	ng	6880	4	11.357	48715	20.0
unknown13.833	13.833	5.0	ng	13640	5	13.992	54548	20.0
unknown14.462	14.462	2.8	ng	7661	5	13.992	54548	20.0
unknown15.121	15.121	7.6	ng	12639	6	15.451	33231	20.0
Benzo[e]pyrene	15.327	5.9	ng	9794	6	15.451	33231	20.0
unknown15.662	15.662	3.1	ng	5220	6	15.451	33231	20.0
Tritetracontane	15.886	8.6	ng	14295	6	15.451	33231	20.0
unknown16.674	16.674	2.7	ng	4535	6	15.451	33231	20.0
unknown16.974	16.974	2.7	ng	4462	6	15.451	33231	20.0
unknown17.221	17.221	2.2	ng	3686	6	15.451	33231	20.0